PREDICTION OF HUMAN INTESTINAL ABSORPTION

By

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Raj Bharatbhai Patel

Dedication

To
My Soulmate Preeti
And
Little Angle Aarushi

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ABSTRACT

The proposed human intestinal absorption prediction model is applied to over 900 pharmaceuticals and has about 82.5% true prediction power. This study will provide a screening tool that can differentiate well-absorbed and poorly-absorbed drugs in the early stage of drug discovery and development. This model is based on fundamental physicochemical properties and can be applied to virtual compounds. The maximum well-absorbed dose (i.e., the maximum dose that will be more than 50 percent absorbed) calculated using this model can be utilized as a guideline for drug design, synthesis, and pre-clinical studies.

CHAPTER 1

INTRODUCTION

New drug discovery and development is unquestionably a very costly process and has no assurance of clinical or commercial success. According to DiMasi *et al.* [1] and Kaitin and DiMasi,[2] the average total cost for developing new chemical entities (NCEs) is almost 800 million dollars and requires decade-long research. On the other hand, the rate at which NCEs are generated is increasing exponentially with the advancement in chemistry and high-throughput screening [3]. Only a small fraction of these synthesized drugs reach the market. Any step that could speed-up this development process will be beneficial. A primary reason for the high attrition of drugs in development is associated with sub-optimal absorption. Predicting human intestinal absorption (HIA) is a challenging task because the absorption of drugs from the gastrointestinal (GI) tract is a complex function of many physicochemical, physiological and pharmaceutical factors, i.e.; solubility, permeability, stability, surface area, pH, pKa, GI blood flow, GI transit time, luminal volume, membrane transport mechanisms and types of dosage forms [4].

Any model that attempts to account for all of these factors will be extremely complicated and not feasible to use in the initial phase of drug discovery. There are various *in vivo* and *in-vitro* models proposed in the scientific literature for predicting human intestinal absorptions. However, many parameters that are required for prediction may not be available in the early stage of drug discovery and development. On the other hand,

computational models are applicable to the design of new drugs [5]. Many computational models utilize a large variety of molecular descriptors, however this may lead to over-fitting which can lower predictability for future compounds. On the other hand, physicochemical property-based computational models are simple and intuitive.

It is well known that solubility and octanol-water distribution coefficient are the two main factors that govern absorption. This work will utilize the intrinsic product as the key driving force that governs human intestinal absorption. Ni *et al.* [6] have shown that this product is equal to the product of the intrinsic solubility and the intrinsic octanol-water partition coefficient. Using the general solubility equation (GSE) [7], the intrinsic product can be replaced by the melting point, which is then a predictor of the steady state absorption rate.

1.1 Background on Physicochemical Properties and Useful Equations Associated with the Proposed Models

Human intestinal drug absorption is a complex process, and it depends on several basic physicochemical properties, such as aqueous solubility, octanol-water partition coefficient, melting point, octanol solubility, pH, pKa, and intrinsic product. In order to understand the proposed models clearly, it is worth reviewing the fundamental relationships among these properties.

1.1.1 Henderson–Hasselbalch Equation

One of the most well-known relationships between pH and pKa is described by the Henderson–Hasselbalch equation. [8]

For weak acids,

$$\mathrm{pH} = \mathrm{pKa} + \log\frac{[\mathrm{A}^-]}{[\mathrm{HA}]} \qquad \text{(Equation 1.1)}$$

where pH is the negative logarithm of the hydrogen ion concentration, pKa is the negative logarithm of the equilibrium constant of a weak acid, [HA] is the molar concentration of the undissociated weak acid, and [A^-] is the molar concentration of the conjugate base.

1.1.2 Ideal Solubility of the Crystalline Solute

Solubility is a very important factor that plays a critical role in drug absorption process, since in order to the drug to be orally absorbed it must be dissolved and available as a solution in GI lumen. Various other key parameters associated with solubility, i.e., dissolution rate, particle size, wettability.

The solubility of a solid in any solvent depends mainly on two factors: the ideal solubility of the crystal and the interaction between the solute and the solvent. According to the Hildebrand and Scott [9] or the Clausius-Clapeyron equation,[10] the ideal solubility, X_u^i, of a crystalline substance can be expressed as

$$\log X_u^i = -\Delta H_m \left(\frac{(T_m - T)}{2.303RTT_m}\right) + \frac{\Delta Cp_m}{2.303R}\left(\frac{(T_m - T)}{T} - \log\frac{T_m}{T}\right) \qquad \text{(Equation 1.2)}$$

where ΔH_m is the molar heat of melting, ΔCp_m is the heat capacity difference between the solid and the molten forms of the solute, R is the gas constant, T and T_m are the room temperature and melting point in Kelvin, respectively.

Ideal solubility is further approximated by assuming ΔCp_m equals zero. [11] Thus

$$\log X_u^i = -\frac{\Delta H_m}{T_m}\left(\frac{T_m - T}{2.303RT}\right)$$ (Equation 1.3)

Since, at the melting point, the Gibbs free energy of melting, ΔG_m, is equal to zero, $\Delta H_m/T_m$ can be replaced by the entropy of fusion, ΔS_m, So

$$\log X_u^i = -\Delta S_m\left(\frac{T_m - T}{2.303RT}\right)$$ (Equation 1.4)

This equation can be further simplified by incorporating Walden's Rule [12] (ΔS_m is 56.5 J/ degree mole for most of the organic molecules)

$$\log X_u^i = -0.01\ (T_m - T\ )$$ (Equation 1.5)

where T and T_m are the room temperature and the melting point in degrees Kelvin, respectively.

The ideal solubility of crystalline solute at the room temperature is

$$\log X_u^i = -0.01\ (MP - 25\ )$$ (Equation 1.6)

where MP is the melting point in degrees Celsius.

1.1.3 Octanol-Water Partition Coefficient

The octanol-water partition coefficient is simply defined as

$$\mathrm{K_{ow}} = \frac{\mathrm{a_o}}{\mathrm{a_w}} \qquad \text{(Equation 1.7)}$$

where a_o and a_w are the activities of a solute in octanol and water, respectively.

Assuming there is no self-association of the solute in either phase and a negligible effect of mutual saturation of the phases, the K_{ow} can be approximated by the solubility ratio of the two phases

$$\mathrm{K_{ow}} = \frac{\mathrm{S_o}}{\mathrm{S_w}} \qquad \text{(Equation 1.8)}$$

In logarithmic terms,

$$\log \mathrm{K_{ow}} = \log \mathrm{S_o} - \log \mathrm{S_w} \qquad \text{(Equation 1.9)}$$

For compounds that are completely miscible with octanol, Jain and Yalkowsky (2001) [7] proposed that the logarithmic octanol solubility can be approximated as a mole fraction value of 0.*5.* Pure octanol is 6.3 molar, and if a solute of similar size is miscible with octanol, it should have a solubility of at least 3.15 molar. Replacing $\log S_o$ with 0.5, which is the logarithm of 3.15, in the above equation gives the aqueous solubility of liquid nonelectrolytes (S_w^L).

$$\log S_w^L = 0.5 - \log K_{ow} \qquad \text{(Equation 1.10)}$$

1.1.4 General Solubility Equation (GSE)

According to Yalkowsky, [7] the solubility of a crystal in water is equal to the solubility of the liquid in water multiplied by the ideal solubility of the crystalline solute. Thus

$$\log S_w^C = \log S_w^L + \log X_u^i \qquad \text{(Equation 1.11)}$$

The GSE is generated by substituting Equation 1.6 and 1.10 into Equation 1.11.

$$\log S_w = 0.5 - \log K_{ow} - 0.01\,(MP - 25) \qquad \text{(Equation 1.12)}$$

The GSE requires only the octanol-water partition coefficient and the experimental melting point to predict the aqueous solubility of a crystalline nonelectrolyte.

1.1.5 Intrinsic Product

A newly defined parameter, the intrinsic product, is the product of the intrinsic solubility and the intrinsic partition-coefficient, therefore

Intrinsic product = $S_w * K_{ow}$

This product can be explained in the term of the GSE by rearranging Equation 1.12. Hence

$$\log S_w + \log K_{ow} = 0.5 - 0.01(MP - 25) \quad \text{(Equation 1.13)}$$

Solving for the Intrinsic product,

$$\log(S_w * K_{ow}) = 0.75 - 0.01(MP) \quad \text{(Equation 1.14)}$$

As per Equation 1.15, this product can also be expressed as a function of melting point

Intrinsic product = $(S_w * K_{ow}) = 10^{0.75-0.01(MP)}$ (Equation 1.15)

By applying the solubility ratio approximation for the octanol-water partition coefficient (Equation 1.8), the intrinsic product can also be written as

Intrinsic product = $(S_w * K_{ow}) = (S_w * \frac{S_o}{S_w}) = S_o$ (Equation 1.16)

where S_o is the octanol solubility of the crystalline solute.

According to Sepassi and Yalkowsky [13] and Admire and Yalkowsky, [14] the octanol solubility of a crystalline solute can be described by Equation 1.17 assuming its hypothetical super-cooled liquid is miscible with octanol,

$$\log S_0 = -\Delta S_m \left(\frac{T_m - T}{2.303RT}\right) + 0.5 \quad \text{(Equation 1.17)}$$

It is important to note that this equation is entirely analogous to Equation 1.11 which gives the solubility of the crystalline solute in water instead of octanol. In other words

$$\log S_o^C = \log X_u^i + \log S_o^L \quad \text{(Equation 1.18)}$$

CHAPTER 2

A RULE OF UNITY FOR HUMAN INTESTINAL ABSORPTION: APPLICATION TO DRUGS THAT ARE MARKETED AS SALTS

Summary

In this chapter, the efficiency of human intestinal absorption (HIA) of 59 drugs which are marketed as salts is predicted using the rule of unity. Intrinsic aqueous solubilities and partition coefficients along with the drug dose are used to calculate modified absorption potential (MAP) values. The application of the rule of unity to over 900 pharmaceutical drugs will be discussed in detail in Chapter 3. The MAP values are shown to be related to the fraction of the dose that is absorbed upon oral administration in humans (FA). It is shown that the MAP value can distinguish between drugs that are poorly absorbed (FA <0.5) and those that are well absorbed (FA ≥ 0.5). Inspection of the data as well as a receiver operative characteristic (ROC) plot show that a single critical MAP value can be used for predicting efficient human absorption of drugs. The rule of unity based on simple *in-vitro* data can be used for predicting whether or not a drug will be well absorbed at a given dose.

2.1 Introduction

2.1.1 Absorption Potential

The concept of absorption potential, based solely on *in vitro* data, was first introduced by Dressman *et al.* [1] (1985) to assess the likelihood of an orally administered drug to be well absorbed. Balon *et al.* [2] (1999) defined the human intestinal absorption potential, AP, of a drug as,

$$\mathrm{AP} = \log\left(\frac{\mathrm{S_T^{6.8}} * \mathrm{K_D^{6.8}} * \mathrm{V_L}}{\mathrm{Dose}}\right) \qquad \text{(Equation 2.1)}$$

where $S_T^{6.8}$and $K_D^{6.8}$are the total solubility in water and the octanol-water distribution coefficient, respectively, of the drug at pH 6.8. He showed a correlation between this absorption potential and the fraction absorbed of a series of drugs. If the gastro intestinal (GI) luminal volume (V_L) is assumed to be 0.250 L, this becomes

$$AP = log\left(\frac{S_T^{6.8} * K_D^{6.8}}{4 * Dose}\right) \qquad \text{(Equation 2.2)}$$

Shortly thereafter, Ni *et al.* [3] (2002) showed that the product of the solubility of a compound in water at any pH (S_T^{pH}) and the octanol-water distribution coefficient at the same pH (K_D^{pH}) is equal to the product of the intrinsic solubility (S_w^{int}) and the intrinsic partition coefficient (K_{ow}^{int}), i.e.,

$$S_T^{pH} * K_D^{pH} = S_w^{int} * K_{ow}^{int}$$ (Equation 2.3)

They demonstrated that this relationship is valid over a wide pH range for zwitterions as well as weak acids and weak bases. As illustrated in Figure 2.1, any change in solubility with pH is accompanied by an equal in magnitude and opposite in direction change in partition coefficient. Therefore, the intrinsic product ($S_w^{int} * K_{ow}^{int}$) is the effective driving force for membrane transport. Its constancy greatly facilitates the calculation of the absorption potential by eliminating the need to know the pKa of the compound or the pH of the gastrointestinal tract micro-environment.

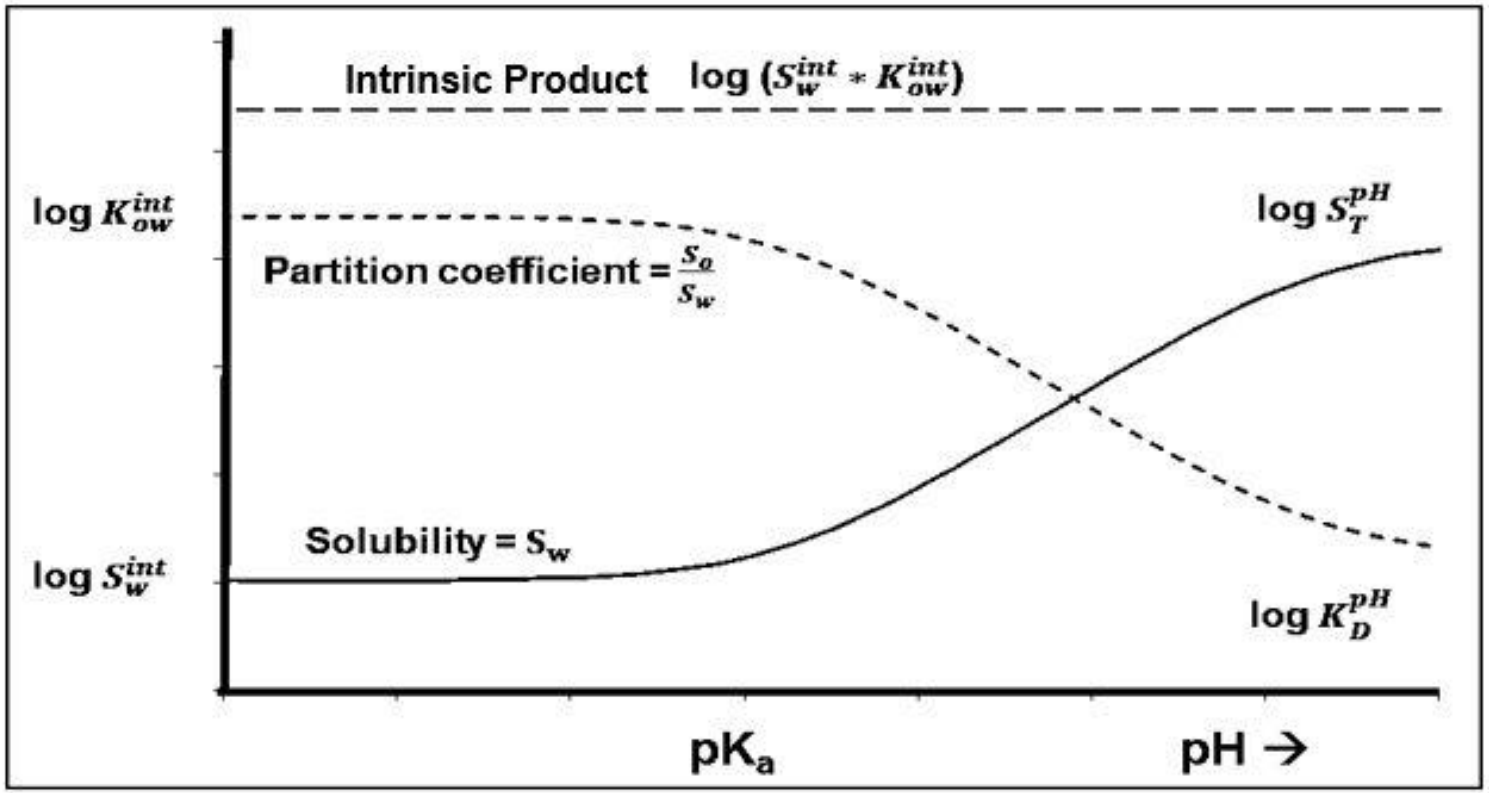

Figure 2.1 Dependence of Solubility, Partition Coefficient, and Their Product as a Function of pH.

2.1.2 Modified Absorption Potential

Replacing the solubility and partition coefficient in Equation 2.1 with the intrinsic product, Sanghvi *et al.* (2001) [4] defined a modified absorption potential as,

$$MAP = log\left(\frac{S_w^{int} * K_{ow}^{int}}{4 * Dose}\right) \quad \text{(Equation 2.4)}$$

If the administered dose is soluble in the 0.250 liters of the GI tract, then the dissolved drug concentration, C_L, is equal to 4* Dose. Therefore,

$$MAP = log\left(\frac{C_L * K_{ow}^{int}}{4 * Dose}\right) = logK_{ow}^{int} \quad \text{(Equation 2.5)}$$

For drugs that are completely dissolved in the GI tract at a given dose, MAP is calculated using Equation 2.5, while Equation 2.4 is used to calculate MAP for drugs that are not completely dissolved at a given dose. (Note, if the dose is in grams, then both the drug concentration and the drug solubility must be in grams per liter.)

Sanghvi *et al.* (2001; 2003) [4, 5], Yalkowsky *et al.* (2006) [6], and Chu and Yalkowsky (2009) [7] have demonstrated that plots of MAP vs. FA are sigmoidal. The FA values can be characterized as either well absorbed (FA ≥ 0.5) or poorly absorbed (FA < 0.5) by the rule of unity, i.e., whether the value of MAP is greater than or less than zero. These studies

were performed on non-electrolyte drugs which were given as suspensions and were reported to be passively absorbed after oral administration.

According to Equation 2.3, the intrinsic product ($S_w^{int} * K_{ow}^{int}$) is the same for an ionized weak electrolyte and its uncharged form. Therefore, whether the drug is in the salt or uncharged form, its absorption is related to its intrinsic product. In this work, the rule of unity is applied to pharmaceutical salts, where MAP values are calculated using the intrinsic product. Therefore, there was no need to know the pH of the microenvironment of the GI tract to predict absorption potential.

2.2 Method

2.2.1 Absorption Data

Experimental values of absorption data for various pharmaceutical salts were obtained from a well-known human intestinal absorption database developed by Hou *et al.* (2007) [8]. In the database, 578 drugs were reported to be absorbed through passive diffusion. However, the current work only focuses on 59 drugs that are marketed as salts and for which experimental fraction absorbed (FA) values are available in the literature. In Table 2.1, the first 29 drugs have dose values such that they form a solution in the GI tract while the rest of the drugs form a suspension in the GI tract. The drug salts and their FA values are listed in Table 2.1.

2.2.2 Dose

Most of the drug doses were collected from the FDA's Maximum Recommended Therapeutic Dose (MRTD) database [9]. This database was chosen because most values in the database were determined from pharmaceutical clinical trials that employed an oral route of exposure. Moreover, most values were normalized for the average adult weighing 60 kg. The MRTD values which were in mg/kg were converted into mol/60kg dose. If the dose was not available in the database, then the dose listed in either Micromedex [10] or Lexi comp [11] was used. All doses are listed in Table 2.1.

2.2.3 Physical Data

All partition coefficients and intrinsic solubilities were calculated using ACDLABS 9.0 [12]. The primary algorithm for calculating partition coefficients used by ACDLABS is based on the principle of isolating carbons [13]. The algorithm for intrinsic solubility is not published.

2.2.4 Statistical Analysis

To predict whether a drug is well absorbed or poorly absorbed, Receiver Operative Characteristic (ROC) analysis was performed. The ROC analysis is a qualitative evaluation tool that can be used for a binary classifier system (“yes” or “no” type outcomes). The ROC curve is a plot of the fraction of true positives out of all positive prediction (sensitivity) vs. the fraction of false positive out of all negative predictions (specificity), at various threshold settings. IBM SPSS version 21 was used to generate the ROC curve with 95% confidence level, assuming a nonparametric distribution [14].

Table 2.1 Data for Pharmaceutical Salts, Experimental FA and, Calculated MAP

No	Drug	Marketed as	FA	log Sw	log Kow	Dose (mg/60kg)	Dose (mol/60 kg)	MAP
1	Acamprosate	Calcium	0.11	0.48	-2.63	1998	1.10E-02	-2.63
2	Anagrelide	Hydrochloride	0.7	-3.3	1.13	10	3.90E-05	1.13
3	Benserazide	Hydrochloride	0.7	-0.27	-2.03	199.8	7.77E-04	-2.03
4	Bethanechol	Chloride	0.05	0.39	-3.95	199.8	1.02E-03	-3.95
5	Carteolol	Hydrochloride	0.95	-1.53	1.35	10.02	3.43E-05	1.35
6	Diethylpropion	Hydrochloride	0.95	-2.47	2.95	75	3.65E-04	2.95
7	Eflornithine	Hydrochloride	0.55	-0.01	0.3	24000	1.32E-01	0.30
8	Etidronate	Disodium	0.05	0.61	-3.53	1200	5.82E-03	-3.53
9	Fenoterol	Hydrobromide	0.6	-1.31	1.09	1.602	5.28E-06	1.09
10	Galantamine	Hydrobromide	0.95	-1.84	1.75	24	8.35E-05	1.75
11	Guanadrel	Sulfate	0.8	-1.48	0.01	400	1.88E-03	0.01
12	Ibutilide	Fumarate	0.82	-3.01	4.17	2	5.20E-06	4.17

13	Ipratropium	Bromide	0.05	-0.21	-2.21	1	3.01E-06	-2.21
14	Levobunolol	Hydrochloride	1	-2.89	2.86	4	1.37E-05	2.86
15	Metaproterenol	Sulfate	0.43	-0.12	0.13	80	3.79E-04	0.13
16	Metformin	Hydrochloride	0.54	0.89	-2.31	3000	2.32E-02	-2.31
17	Methylergonovine	Maleate	1	-2.64	1.68	2	4.71E-06	1.68
18	Methylphenidate	Hydrochloride	0.8	-2.17	2.54	60	2.57E-04	2.54
19	Metoprolol	Tartrate	0.96	-1.41	1.79	400.2	1.50E-03	1.79
20	Mivacurium	Chloride	0	-2.15	0.37	12	1.17E-05	0.37
21	Neomycin	Sulfate	0.03	0.2	-4.41	12000	1.91E-02	-4.41
22	Netilmicin	Sulfate	0	0.32	-2	450	9.46E-04	-2.00
23	Oxitropium	Bromide	0.16	-0.2	-2.36	0.6	1.80E-06	-2.36
24	Pamidronic acid	Disodium	0.05	0.63	-3.4	90	3.83E-04	-3.40
25	Pramipexole	Dihydrochloride	0.8	-1.9	1.42	6	2.84E-05	1.42
26	Propantheline	Bromide	0	-0.35	-1.77	360	9.77E-04	-1.77
27	Risedronic acid	Sodium	0.01	-0.23	-2.94	4.998	1.77E-05	-2.94
28	Sotalol	Hydrochloride	0.95	-0.84	0.94	319.8	1.17E-03	0.94
29	Timolol	Maleate	0.95	-2.14	0.06	60	1.90E-04	0.06

30	Cefmetazole	Sodium	0.1	-5.26	0.97	6000	1.27E-02	-3.00
31	Cefotaxime	Sodium	0.05	-4.5	1.28	12000	2.63E-02	-2.24
32	Chlorpromazine	Hydrochloride	0.98	-5.26	4.82	1002	3.14E-03	1.46
33	Clindamycin	Hydrochloride	0.87	-1.96	1.83	1800	4.24E-03	1.64
34	Diatrizoate	Sodium	0.05	-3.12	0.45	29040	4.57E-02	-1.93
35	Dolasetron	Mesylate	0.85	-3.69	2.82	100	3.08E-04	2.04
36	Ergotamine	Tartrate	1	-5.22	3.58	6	1.03E-05	2.74
37	Estramustine	Phosphate	0.75	-6.47	5.35	960	2.18E-03	0.94
38	Flunarizine	Hydrochloride	0.8	-5.01	5.02	150	3.69E-04	2.84
39	Fluorescein	Sodium	0.99	-4.9	2.98	1500	4.51E-03	-0.18
40	Fluoxetine	Hydrochloride	0.8	-3.66	4.09	79.8	2.58E-04	3.42
41	Fluvoxamine	Maleate	0.9	-2.91	3.11	300	9.42E-04	2.62
42	Guanabenz	Acetate	0.78	-3.28	2.57	96	4.15E-04	2.07
43	Imatinib	Mesylate	0.98	-4.32	2.48	800	1.62E-03	0.35
44	Imipramine	Palmonate	0.98	-4.61	4.8	300	1.07E-03	2.56
45	Lomefloxacin	Hydrochloride	0.99	-4.23	2.37	400	1.14E-03	0.48
46	Maprotiline	Hydrochloride	0.98	-4.33	4.51	225	8.11E-04	2.67

47	Mefloquine	Hydrochloride	0.78	-3.29	2.76	1250	3.30E-03	1.35
48	Mezlocillin	Sodium	0	-3.6	-1.18	16020	2.97E-02	-3.85
49	Mianserin	Hydrochloride	0.7	-4.26	3.67	90	3.40E-04	2.28
50	Nefopam	Hydrochloride	0.98	-2.56	3.44	300	1.18E-03	3.20
51	Propafenone	Hydrochloride	0.95	-3.61	3.93	900	2.64E-03	2.30
52	Protriptyline	Hydrochloride	0.95	-3.94	5.06	60	2.28E-04	4.16
53	Quetiapine	Fumarate	0.73	-3.58	1.57	798	2.08E-03	0.07
54	Tacrine	Hydrochloride	0.95	-3.36	2.63	160	8.07E-04	1.76
55	Terbinafine	Hydrochloride	0.8	-6.35	6.61	1620	5.56E-03	1.91
56	Tiagabine	Hydrochloride	0.9	-4.86	5.68	64.2	1.71E-04	3.99
57	Ticlopidine	Hydrochloride	0.8	-3.79	3.77	250.2	9.48E-04	2.40
58	Tolazoline	Hydrochloride	0.9	-2.74	2.65	120	7.49E-04	2.43
59	Tolmetin	Sodium	0.99	-2.59	1.55	1800	7.00E-03	0.51

2.3 Results and Discussion

Figure. 2.2 shows the plot of FA vs. MAP for the 59 salts studied. The figure is divided into four quadrants. The points in the upper right (True Positive) and lower left (True negative) represent correct predictions of high and low absorption efficiency. The points in the lower right (False positive) and upper left (False negative) quadrants represent incorrect predictions. Also, the prediction power of this model is more accurate when the MAP value is higher than 2 or lower than -2. The MAP is a simple absorption parameter which is a good indicator of absorption efficiency of salts, and there is no need to know about the total solubility, distribution coefficient or dissociation constant of the drug.

In Figure 2.2, the rule of unity is represented by the bold vertical line which is a simple delineator that can differentiate between poorly absorbed and well-absorbed drugs. A more appropriate delineator value for this data set was found using ROC curve analysis. As described earlier, the ROC curve analysis can be used to determine the most appropriate cut-off value for a set of binary data, i.e., data that can be represented as yes or no. Therefore, it can be used to distinguish between poorly absorbed and well-absorbed drugs. Using calculated MAP values, a ROC curve, (Figure 2.3), was created to determine the MAP value that has the highest model sensitivity (Probability of finding high MAP values when good absorption has been reported) and specificity (Probability of finding low MAP values when poor absorption has been reported).

The ROC curve was generated by plotting the calculated sensitivity on the Y-axis and plotting the calculated 1- specificity on the X-axis. The sensitivity and specificity were calculated by

$$\text{Sensitivity} = \frac{\#\text{ of correct positive predictions}}{\text{Total }\#\text{ of positive predictions}}$$

and

$$\text{Specificity} = \frac{\#\text{ of correct negative predictions}}{\text{Total }\#\text{ of negative predictions}}$$

respectively.

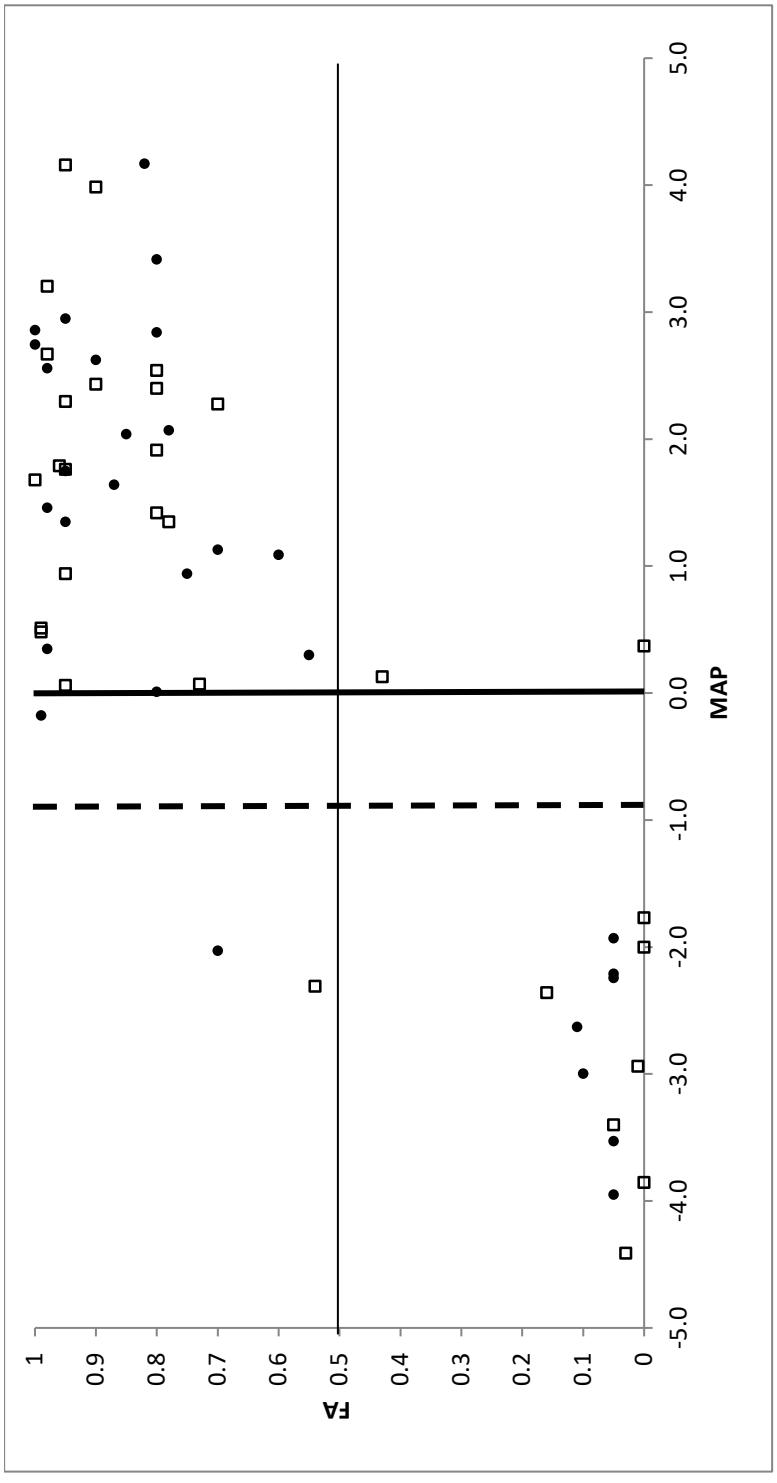

Figure 2.2 Fraction Absorbed vs. MAP for Drugs That Are Administered as Salts.

□ Calculated by Equation 2.4, ● : Calculated by Equation 2.5.

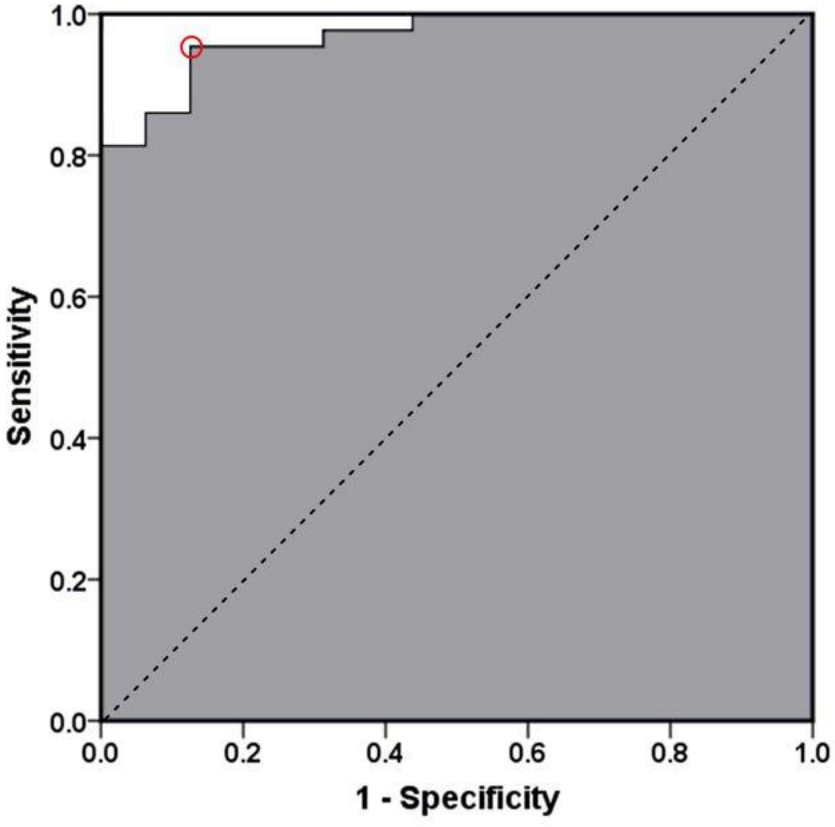

Figure 2.3 ROC Plot for MAP.

In Figure 2.3, the circle represents the maximum product of the sensitivity (0.953) and specificity (0.875). This point corresponds to best delineating MAP value which is -0.973. This new value, which is represented by a dashed line in Figure 2.2 is statistically more accurate than zero and may be used as a new delineator for the rule of unity. In other words, if the calculated MAP value is higher than -0.973, it is more likely that the drug is well absorbed. The shaded fraction of the ROC curve, approximately 0.968, which can be considered approximately analogous to the R-square value of a regression line, confirms the strength of this model.

The human intestinal absorption results for the salts studied are summarized in Table 2.2. Clearly, there is a good correlation between the observed FA and predicted MAP values for the whole data set as well as subsets. The cut-off value of zero is used to differentiate well-absorbed and poorly absorbed compounds in this model.

Overall, 91.5% of the predictions of this model are correct. The above results are further confirmed by the data of Avdeef *et al.* (2008) [15]. They studied the effect of accurately measured solubility and an artificial membrane permeability (PAMPA), on the absorption of sparingly soluble drugs. They observed that at a high dose, where the drug is not completely dissolved, the absorption flux is constant as the pH-permeability, and pH-solubility curves mirror each other. They also observed that at a low dose where the drug is completely dissolved, the absorption flux is a function of the effective permeability.

Table 2.2 Human Intestinal Absorption Prediction Results for Salts

Category	**True Prediction**	**False Prediction**	**Total**
Solution (4D $\leq$ Sw)	25	4	29
Suspension (4D > Sw)	29	1	30
All	54	5	59

2.4 Conclusion

The absorption efficiency of salts can be characterized based on a simple MAP value which is a function of the drug dose and calculated or observed aqueous solubilities and partition coefficients. However, this calculation is solely based on physical data and may not account for physiological conditions along the GI tract or dissolution kinetics of drug formulations.

If the value of the MAP is greater than zero, the salts are generally well (> 50%) absorbed, and if it is less than zero, the salts tend to be poorly absorbed. The human intestinal absorption was predicted correctly for 54 out of total 59 salts used in this model. Thus, the rule of unity could be utilized as a pre-screening tool for predicting human intestinal absorption for orally administered drugs.

CHAPTER 3

A RULE OF UNITY FOR HUMAN INTESTINAL ABSORPTION: APPLICATION TO PHARMACEUTICALS

Summary

The rule of unity is based on a simple absorption parameter, Π, that can accurately predict whether an orally administered drug will be well absorbed or poorly absorbed. In this chapter, the intrinsic aqueous solubility and octanol-water partition coefficient, along with the drug dose are used to calculate Π. We show that a single delineator value for Π exists that can distinguish whether a drug is likely to be well absorbed (FA ≥ 0.5) or poorly absorbed (FA < 0.5) at any specified dose. The model is shown to give 82.5 percent correct predictions for over 938 pharmaceuticals. The maximum well-absorbed dose (i.e., the maximum dose that will be more than 50 percent absorbed) calculated using this model can be utilized as a guideline for drug design and synthesis.

3.1 Introduction

New drug discovery and development is unquestionably a very costly process, with only a small fraction of synthesized drugs reaching the market. According to DiMasi *et al.* [1] and Kaitin and DiMasi [2], in 2011, the average total cost for developing new chemical entities (NCEs) is almost 800 million dollars and requires decades-long research. The primary reason for the high attrition of drugs in development is associated with sub-optimal absorption.

Predicting human intestinal absorption (HIA) is a challenging task because the absorption of drugs from the gastrointestinal (GI) tract is a complex function of many physicochemical, physiological and pharmaceutical factors. Including; drug solubility, permeability, pKa, dose, GI luminal volume, and pH. [4] The proposed simple and intuitive approach uses only the aqueous solubility, octanol-water partition coefficient, and dose of the drug as input.

3.1.1 Membrane Transport Model

The transport rate (or flux) of a drug from the GI lumen through the GI membrane into the blood can be described by the physical model of Stehle and Higuchi (1972) [15], i.e.,

$$F \propto \Delta C \times K_{ow} \qquad \text{(Equation 3.1)}$$

where F is the flux from a solution, ΔC is the concentration difference between the gut and the blood, and K_{ow} is the membrane-water partition coefficient of the drug which is assumed to be identical to the octanol-water partition coefficient.

3.1.2 Absorption Potential

In 1985, Dressman *et al.* [16] introduced the concept of absorption potential. Using *in vitro* data for seven drugs, they showed the interrelation of drug dose, partition coefficient, and solubility to the fraction of the dose absorbed. They defined the absorption potential, $\mathrm{AP_{Dressman}}$, as,

$$\mathrm{AP_{Dressman}} = \log\left(\frac{\mathrm{K_{ow}} * \mathrm{F_{non}} * \mathrm{S_w^{int}} * \mathrm{V_L}}{\mathrm{D}}\right) \qquad \text{(Equation 3.2)}$$

where, $\mathrm{F_{non}}$ is the fraction in the nonionized form at pH 6.5, $\mathrm{S_w^{int}}$ is the intrinsic solubility of the nonionized species at 37°C, D is the dose administered, and $\mathrm{V_L}$ is the intestinal luminal volume.

Balon *et al.* [17] (1999) further developed the human intestinal absorption potential model by modifying the numerator of the above equation so that the solubility and the partition coefficient both reflect the same physiological pH, i.e.,

$$\mathrm{AP_{Balon}} = \log\left(\frac{\mathrm{S_T^{6.8}} * \mathrm{K_D^{6.8}} * \mathrm{V_L}}{\mathrm{D}}\right) \qquad \text{(Equation 3.3)}$$

where $S_T^{6.8}$and $K_D^{6.8}$are the solubility in water and the octanol-water distribution coefficient, respectively, of the drug at pH 6.8.

If the gastrointestinal (GI) luminal volume (V_L) is assumed to be 0.250 L, and the drug is not completely dissolved, we can define the absorption potential of a suspension, AP_{susp}, as

$$AP_{susp} = \log\left(\frac{S_T^{6.8} * K_D^{6.8}}{4D}\right) \quad \text{(Equation 3.4)}$$

3.1.3 Intrinsic Product

Ni *et al.* [6] (2003) observed an important relationship between the pH, partition coefficient, and solubility. They showed that the product of the total solubility of a compound in water at any pH (S_T^{pH}) and the octanol-water distribution coefficient at the same pH (K_D^{pH}) is equal to the product of the intrinsic solubility (S_w^{int}) and the intrinsic partition coefficient (K_{ow}^{int}), i.e.,

$$S_T^{pH} * K_D^{pH} = S_w^{int} * K_{ow}^{int} \quad \text{(Equation 3.5)}$$

Note, that the above equation assumes that salt precipitation and ion pair partitioning are not significant. They demonstrated that this relationship was valid for 25 compounds comprising zwitterions as well as weak acids and weak bases over a wide pH range.

Therefore, the intrinsic product ($\mathrm{S_w^{int}} * \mathrm{K_{ow}^{int}}$) is the effective driving force for membrane transport. Its constancy greatly facilitates the calculation of the human intestinal absorption by eliminating the need to know the pKa of the compound or the pH of the gastrointestinal tract microenvironment.

3.1.4 Modified Absorption Potential

Sanghvi *et al.* [18] (2001) introduced the modified absorption potential by replacing the solubility and partition coefficient with the intrinsic product, therefore,

$$\mathrm{MAP}_{susp} = \log\left(\frac{\mathrm{S_w^{int}} * \mathrm{K_{ow}^{int}}}{4\mathrm{D}}\right) \qquad \text{(Equation 3.6)}$$

where MAP_{susp} is the modified absorption potential for an incompletely dissolved drug. This eliminates the need to know the pK_a of the drug or the pH of the luminal microenvironment. In addition, the experimentally measured intrinsic values are more reliable than fixed pH measurements.

Later Sanghvi *et al.* [19] (2003) showed that the MAP model could be divided broadly into two categories based on whether the orally administered dose forms a solution or a suspension in the gut.

3.1.4.1 Drugs that form solutions at their administered dose (4D $\leq$ Sw)

If the drug is completely soluble in the volume of GI luminal fluid, then the aqueous solubility, S_w, can be replaced by the concentration of the drug in the GI luminal fluid, C_L. Typically, this volume is assumed to be 0.25 L. Thus, for any dose that can be dissolved completely in 0.25L of the GI fluid,

$$\mathrm{Sw} = \frac{\mathrm{D}}{0.25} = 4\mathrm{D} \qquad \text{(Equation 3.7)}$$

therefore, the MAP values for a solution can be calculated simply by replacing $\mathrm{S_w^{int}}$ in Equation 3.6 with 4D.

$$\mathrm{MAP_{Sol}} = \log\left(\frac{4\mathrm{D}*\mathrm{K_{ow}^{int}}}{4\mathrm{D}}\right) = \log\mathrm{K_{ow}^{int}} \qquad \text{(Equation 3.8)}$$

3.1.4.2 Drugs that forms suspensions at their administered dose (4D > Sw)

Drugs that do not dissolve completely in the volume of aqueous GI luminal fluid form a suspension in the gut. Thus, assuming the drug does not form a supersaturated solution, the maximum dose that can be dissolved is equal to its intrinsic solubility. The MAP values for a suspension can be calculated using the equation below,

$$\mathrm{MAP_{Susp}} = \log\left(\frac{\mathrm{S_w^{int}}*\mathrm{K_{ow}^{int}}}{4\mathrm{D}}\right) \qquad \text{(Equation 3.9)}$$

For slightly supersaturated solution this is only true for the initial phase until the supersaturated solution becomes a true solution. (Note that if the dose is in grams, then both the drug concentration and the drug solubility must be in grams per liter)

3.1.5 Luminal Oversaturation Number and Development of Absorption Parameter Π

Sanghvi *et al.* [19] (2003) introduced the rule of unity and developed a new unitless parameter called luminal oversaturation number, O_{Lumen}, which reflects the degree of oversaturation of the GI luminal fluid by drugs. It is defined as,

$$O_{Lumen} = \max\left(\frac{4D}{S_w^{int}}, 1\right) \qquad \text{(Equation 3.10)}$$

Thus, the luminal oversaturation number offers a convenient means to differentiate high and low solubility drugs. It is defined similarly to the dose number. However, it cannot be less than unity. Daousani and Macheras [20] observed that the ratio of dose to solubility is not a constant parameter and it is a key driving force in the drug dissolution process.

Using O_{Lumen}, they developed a more intuitive absorption parameter, Π, which is the logarithmic ratio of the partition coefficient and the unitless oversaturation number. This parameter applies to both suspended and dissolved drugs.

$$\Pi = \log\left(\frac{K_{ow}^{int}}{O_{Lumen}}\right) = MAP_{sol} - \log O_{Lumen} = MAP_{susp} \qquad \text{(Equation 3.11)}$$

It is worth noting that the absorption parameter Π (Equation 3.11), becomes either Equation 3.8 or Equation 3.9, based on the whether the drug is forming a solution or a suspension in the GI tract at the administered dose. The above results are further confirmed by the data of Avdeef *et al.* [21] They studied the effect of accurately measured solubility and an artificial membrane permeability (PAMPA) model, on the absorption of sparingly soluble drugs. Their data show that at a high dose, where the drug is not completely dissolved, the absorption flux is constant as the pH-permeability, and pH-solubility curves mirror each other. Their data also show that at a low dose where the drug is completely dissolved, the absorption flux is a function of the effective permeability.

3.1.6 Human intestinal absorption and membrane transport mechanisms

The small intestine acts as the main absorption site for many orally administered drugs. As shown in Figure 3.1, these drug molecules can cross human intestinal membrane by one or more of following mechanisms; passive diffusion, facilitated diffusion, paracellular transport, transcellular transport, active influx, and active efflux.

Passive diffusion is energy independent and concentration gradient based transfer of drug molecules across the membrane. In other words, the drug molecules move across the cell membrane from a high concentration to a low concentration. This process is mainly governed by Fick's first law. i.e.,

$$\frac{dn}{dt} = D\ A\ P\ \frac{dC}{dX} \qquad \text{(Equation 3.12)}$$

where $\frac{dn}{dt}$ is the rate of diffusion, D is the diffusion coefficient, A is the surface area of the membrane, P is the permeability, $\frac{dC}{dX}$ is the concentration gradient across the membrane. Venous blood is continuously flowing which maintains sink conditions across the cell membrane. This condition is a driving force for the passive diffusion. [22-25]

Facilitated diffusion is a passive transport in which drug molecule is diffused via specific transmembrane proteins. In paracellular transport, the drug molecule is carried by passing through the space between the enterocyte cells. This route is more selective for small (MW<200), hydrophilic (logK_{OW}<0), cationic drugs due to the characteristic water pores and tight junctions [23,26]. In transcellular transport, the drug molecule permeates the apical membrane of the enterocyte, diffuses through the cell, and diffuses out through the basolateral membrane to be absorbed into the blood. The transcellular transport comprises of transcellular diffusion, endocytosis, exocytosis, and/or active carrier mediated transcellular transport. [22,23]

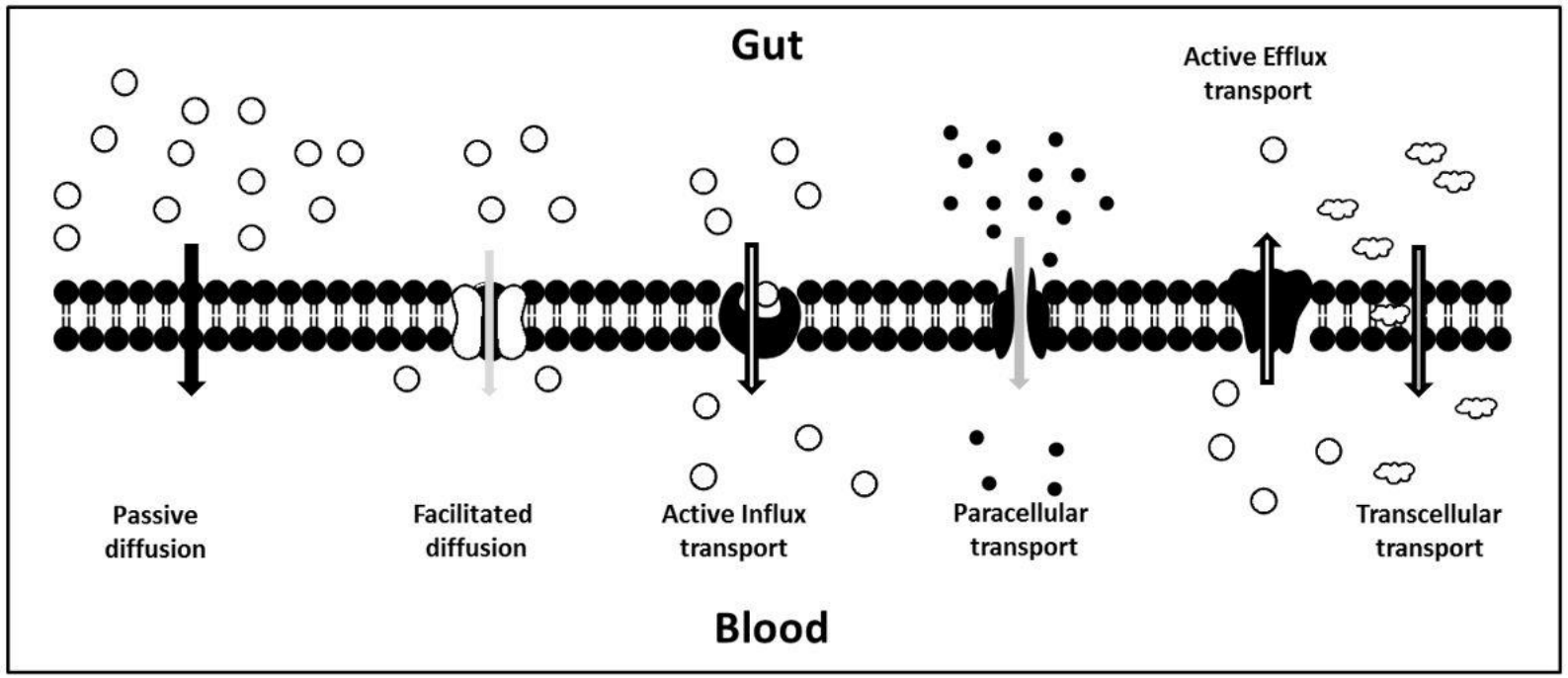

Figure 3.1 Membrane Transport Mechanisms.

The process of active transport is energy dependent and against the concentration gradient. In other words, the drug molecules move across the cell membrane from lower concentration to higher concentration. In a nutshell, the process of active influx means transporters on the membrane increase the drug concentrations into the cell, and active efflux transport means transporters on the membrane decrease the drug concentrations inside the cell. Both influx and efflux transporters are important in drug design. Many researchers suggest that the drug absorption can be improved by manipulating active influx transporters. [27-29] Some researchers indicate that drug absorption can also be improved by avoiding potential substrate of efflux transporters. [30,31] It is worth mentioning that compared to passive transport carrier-mediated active transport can be quickly saturated. There are two different opinions regarding drug transport mechanisms. According to one group, multiple absorption mechanisms coexist for the oral absorption [32-34] According to another group, all drug absorption is solely mediated by transporters. [27,35,36]

3.2 Method

3.2.1 Compound selection

The rule of unity model by Sanghvi *et al.* [19] and Yalkowsky *et al.* [37] only applies to nonelectrolyte drugs which were reported to be passively absorbed after oral administration. To make a more robust and a more generalized model, we have incorporated all kinds of pharmaceuticals including salts, nonelectrolytes, or drugs that are reported to undergo active influx or efflux.

3.2.2 Fraction Absorbed Data

Experimental values of oral absorption for a diverse group of pharmaceuticals were obtained from the well-known critically evaluated human intestinal absorption databases developed by Hou *et al*. [38], Newby *et al.* [39] and other scientific literature. [3,19,40] When FA values were reported as a range or when more than one value was reported; the mean value was adopted in this database. The fraction absorbed data are given in supplementary information in Table A.1 along with the physical property data and the Maximum Recommended Therapeutic Dose (MRTD) values for each compound. It is noted that the reported FA values are skewed towards being well-absorbed because poorly absorbed results are often not reported in the literature.

3.2.3 Drug dose data

Most of the drug doses were collected from the FDA's MRTD database. [41] This database was chosen because most of its values were determined from the results of pharmaceutical clinical trials. Moreover, these values are normalized for the average adult weighing 60 kg. If the dose was not available in the database, then the dose listed in Micromedex [42], Lexicomp [43], Newby *et al.* [39], or other scientific literature [44-54] was used. The relationship between FA and dose is depicted in Figure 3.2. The doses used formed a continuous, well-distributed dataset (8-log distribution) and there is no clear way one can separate the well-absorbed and poorly absorbed compounds solely based on their dose value.

3.2.4 Physicochemical properties

In order to eliminate any bias, all physicochemical properties used in the proposed model were collected from chemical abstract service – SciFinder [55] which were calculated using ACDLABS 11.02 [56] software. If values were not available in SciFinder, then ACDLAB 7.0 [57] software was used to calculate all physicochemical properties. The group contribution methods like UPPER can also be utilized to calculate some physicochemical properties (Chapter 5).

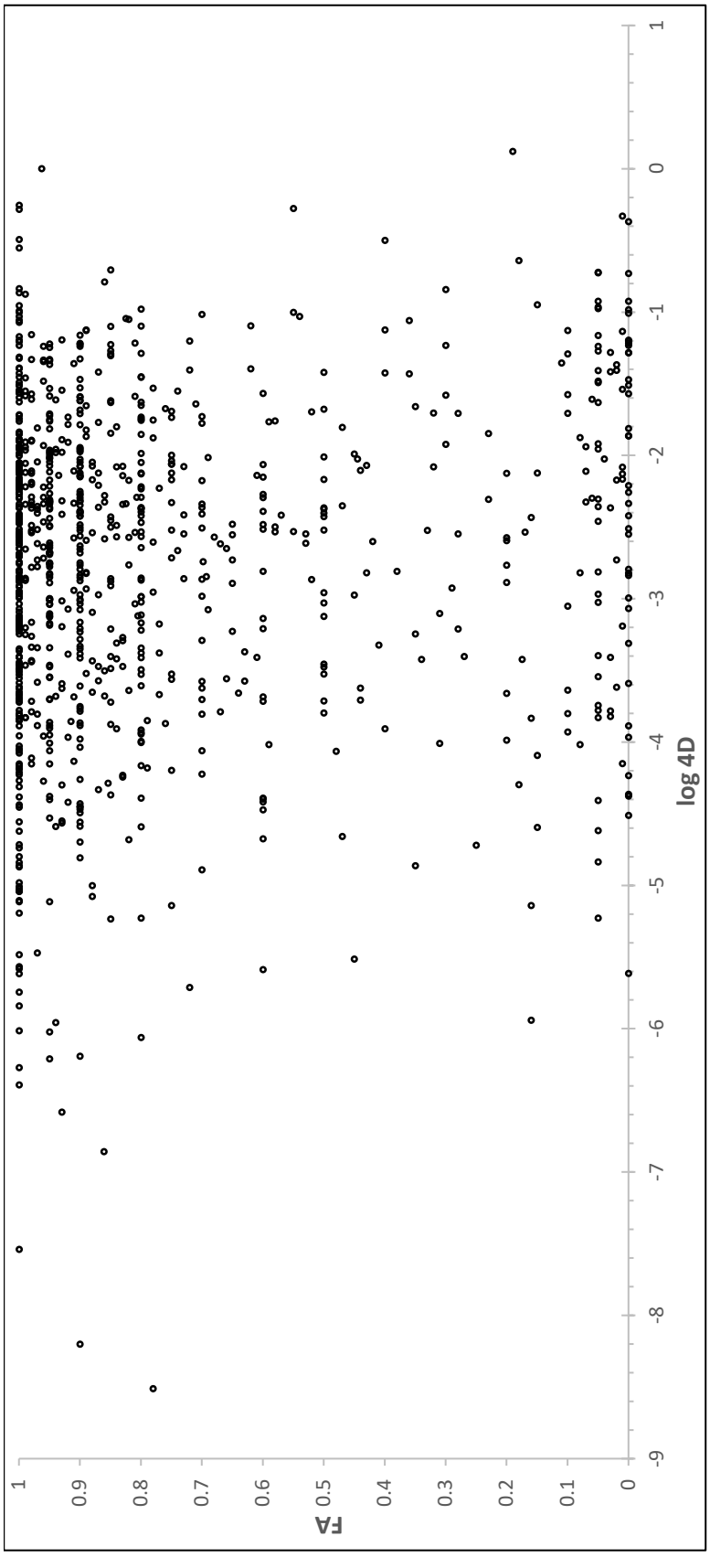

Figure 3.2 Relationship Between the Fraction Absorbed vs. log 4D.

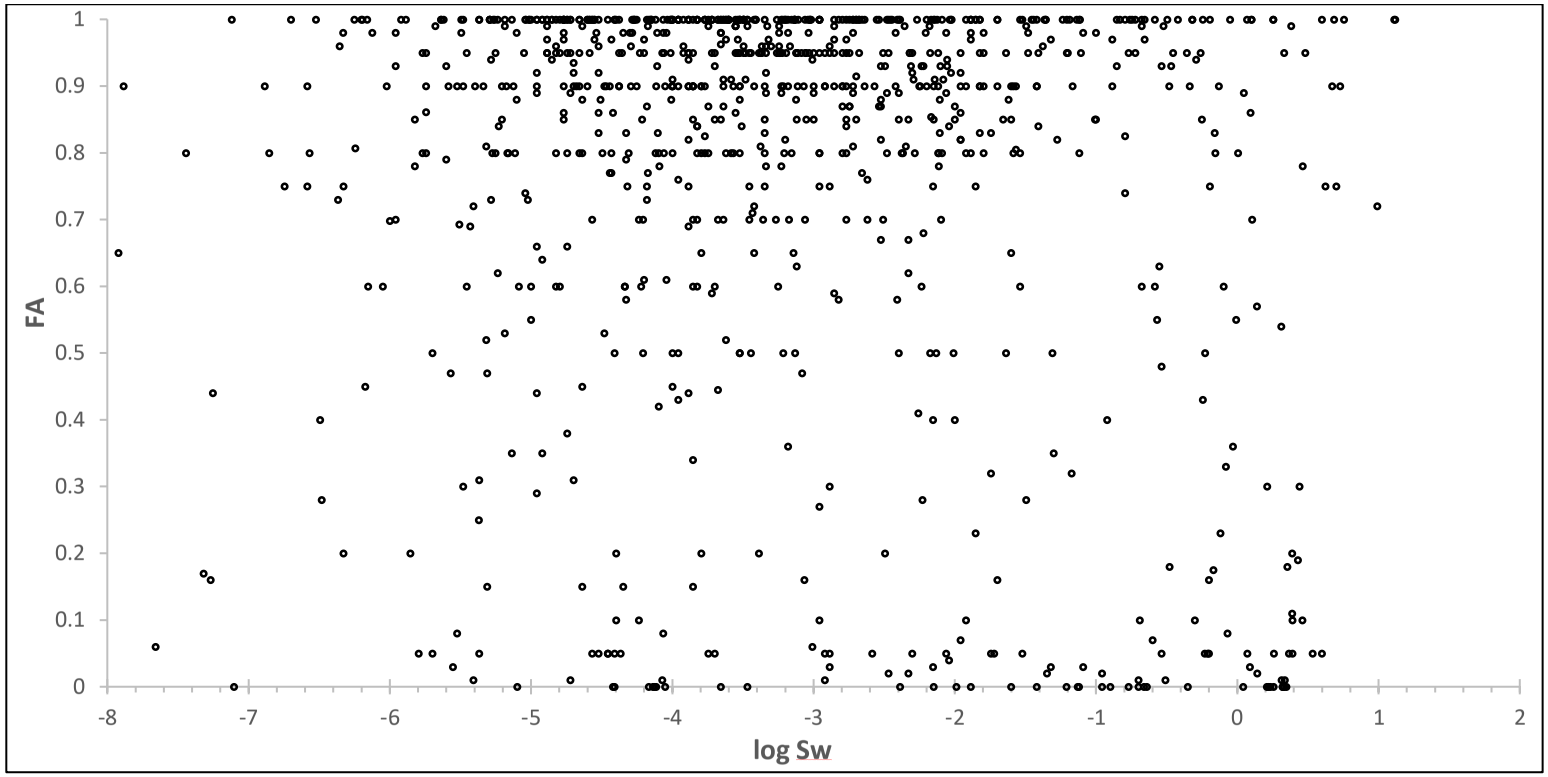

Figure 3.3 Relationship Between the Fraction Absorbed vs. log S_w.

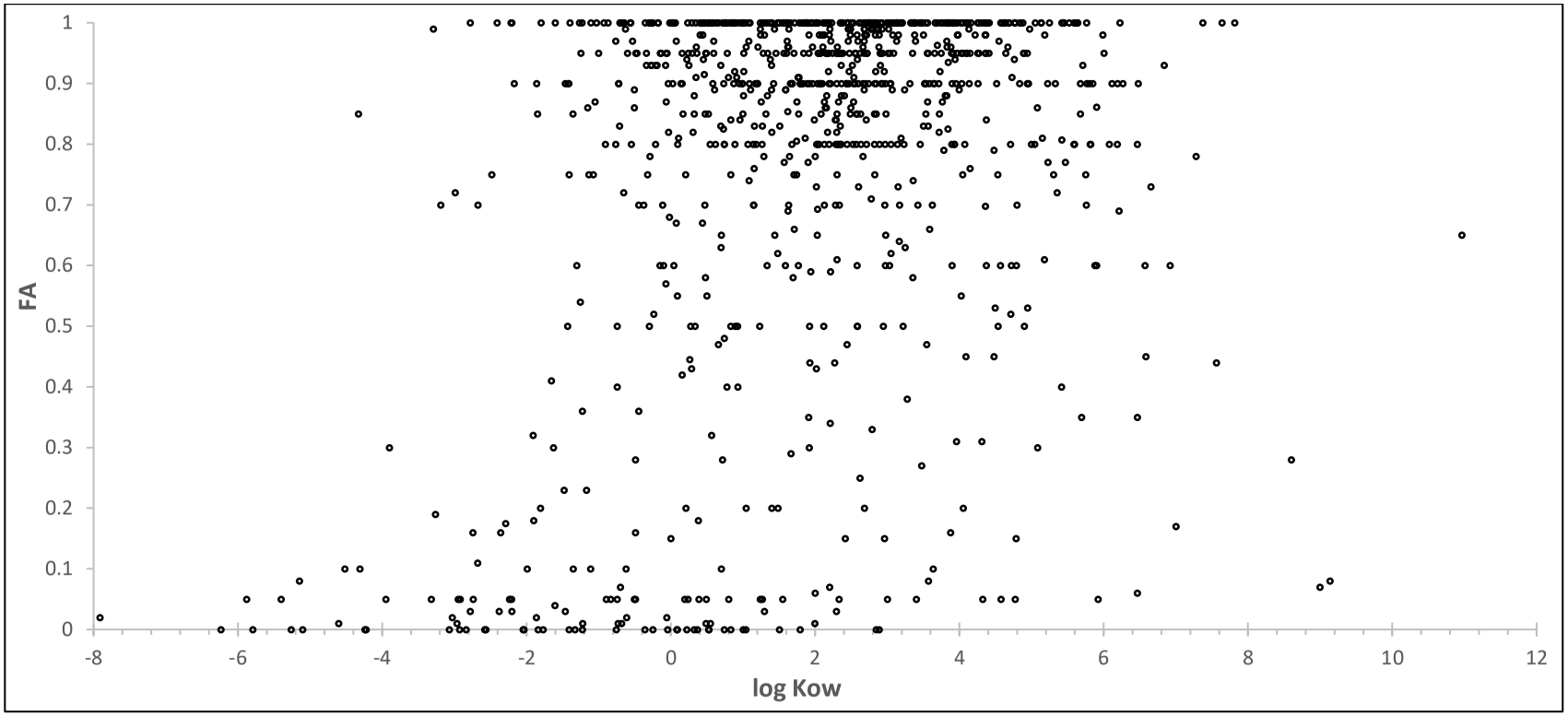

Figure 3.4 Relationship Between the Fraction Absorbed vs. log K_{ow}.

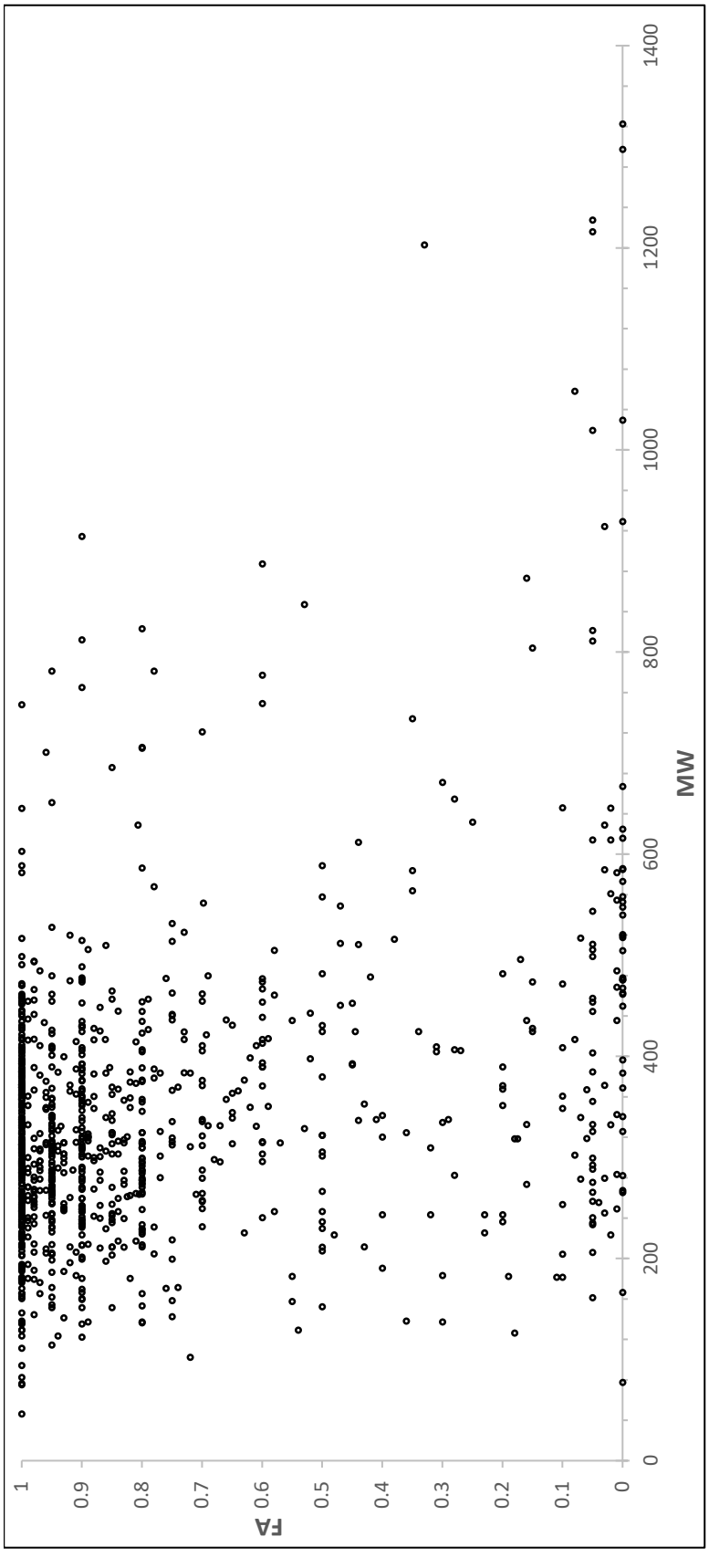

Figure 3.5 Relationship Between the Fraction Absorbed vs. MW.

3.2.5 Calculation of Π

The intrinsic aqueous solubility and octanol-water partition coefficient, along with the maximum recommended therapeutic dose (MRTD) are used to calculate the absorption parameter Π. Although Π can be used to calculate any fraction absorbed, it is most accurate at FA = 0.5.

The proposed human intestinal absorption model is a true *in silico* model as the Π values are predicted only based on calculated partition coefficient and calculated intrinsic solubility using ACDLAB software. This work will reaffirm the relationship between the intrinsic product ($S_w^{int} * K_{ow}^{int}$) and the dose and the experimental values of human intestinal absorption. (Note, that Sanghvi *et al.* used some log S_w values that were experimentally determined, and some that were calculated from the general solubility equation [7].

3.2.6 Statistical Analysis

Addinsoft XLSTAT version18.06 [58] was used to generate the ROC curve with 95% confidence level, assuming a nonparametric distribution.

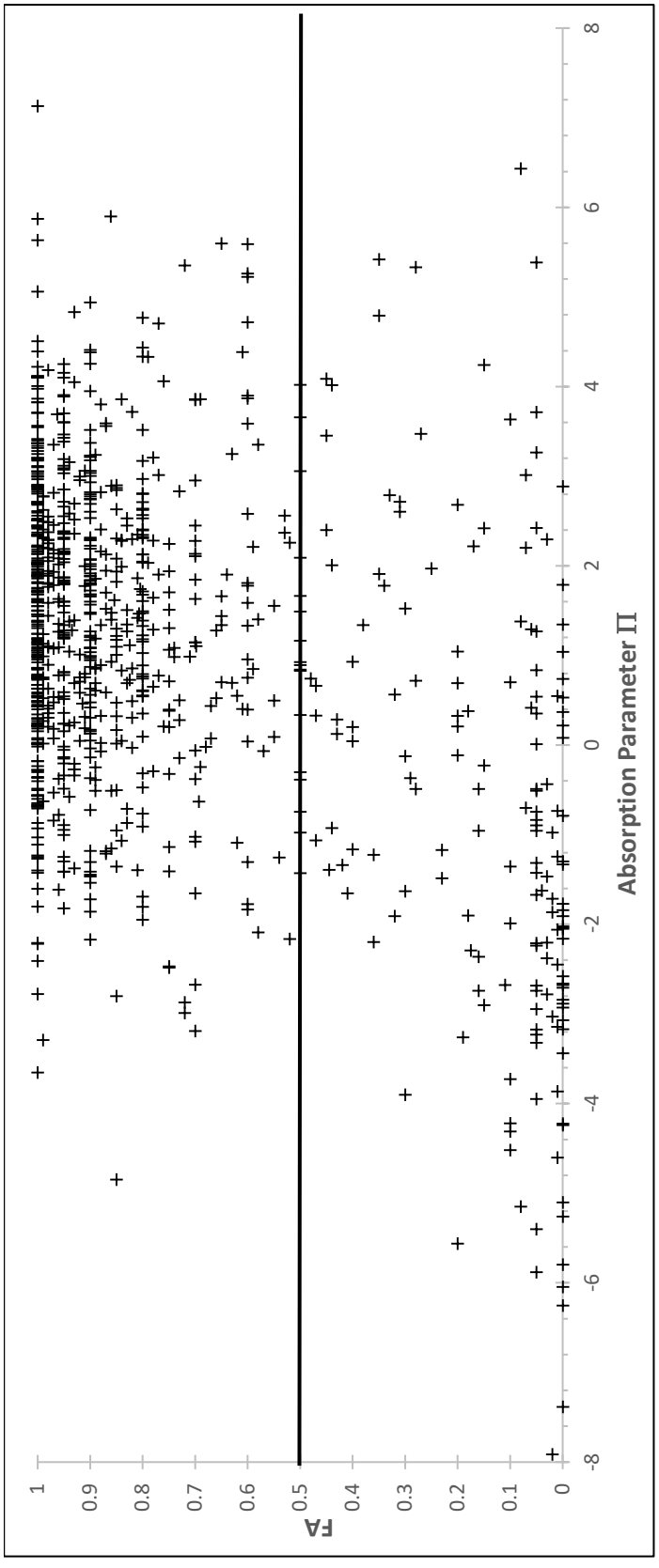

Figure 3.6 Fraction Absorbed vs. Absorption Parameter Π.

3.3 Results and Discussion

The Correlations of the experimental FA values with the physicochemical properties used in this model are shown in Figure 3.2, 3.3, 3.4, and 3.5. It is evident that there is no single vertical delineator line that can differentiate between the pharmaceuticals that are well absorbed from those that are poorly absorbed for any of these properties.

Figure 3.6 is a plot of FA vs. Π for the 938 Pharmaceuticals studied. The horizontal line at FA=0.5 differentiates the well-absorbed (FA≥0.5) and poorly absorbed (FA<0.5) compounds. It is clear that there is a correlation between the fraction absorbed and Π. It is also clear that the relationship between FA and Π cannot be adequately described by a single equation. However, it is possible to define a delineator to separate well-absorbed values from poorly absorbed values. To do this, we utilized Receiver Operative Characteristic (ROC) statistical analysis. The ROC analysis is a qualitative evaluation tool that can be used for a binary classifier system ("yes" or "no" type outcomes). The ROC curve is a plot of sensitivity on the y-axis vs. 1- specificity on the x-axis where

$$\text{Sensitivity} = \frac{\#\text{ of correct positive predictions}}{\text{Total }\#\text{ of positive predictions}} \qquad \text{(Equation 3.13)}$$

and

$$\text{Specificity} = \frac{\text{\# of correct negative predictions}}{\text{Total \# of negative predictions}} \quad \text{(Equation 3.14)}$$

respectively.

The optimum value for Π, is obtained from Youden's index which is defined as

Youden's index = maximum (Sensitivity + Specificity – 1) (Equation 3.15)

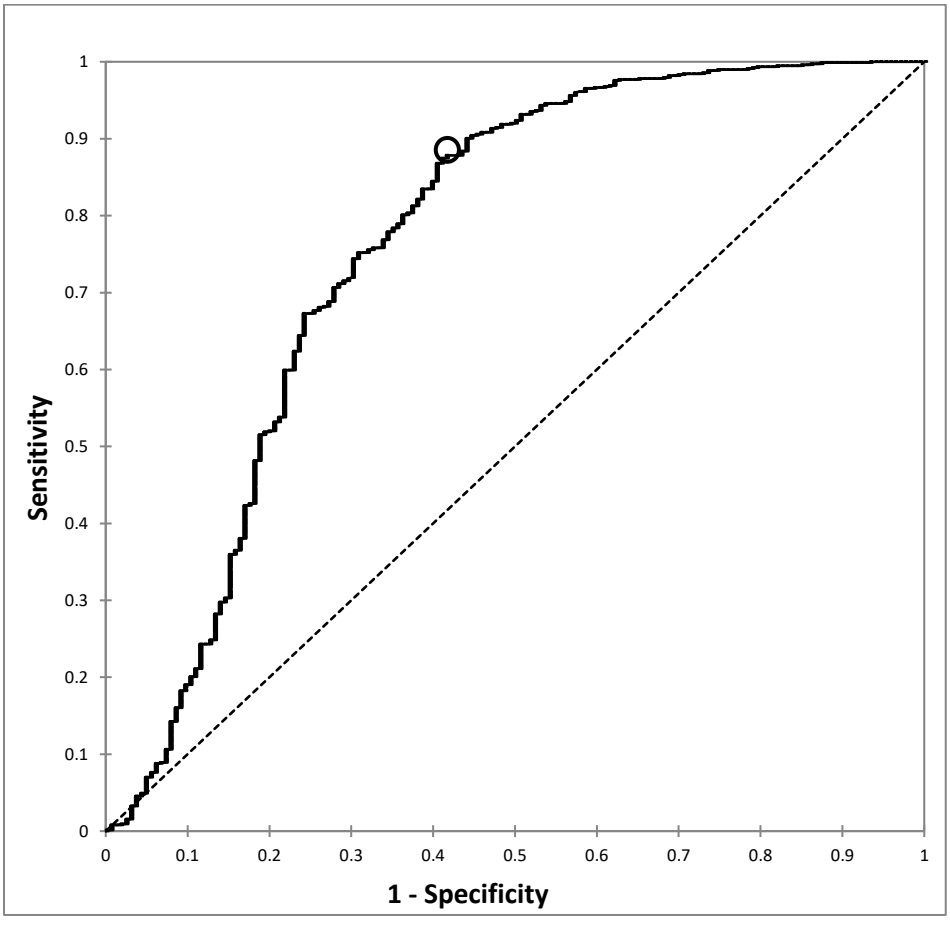

Figure 3.7 The ROC Plot of Sensitivity vs. 1-specificity for Calculating the Delineating Value Π.

This circle in Figure 3.7 is the point that provides the maximum sum of the sensitivity and specificity. It is the farthest point on the plot from the diagonal line between the origin to the point corresponding to both sensitivity and specificity being equal to unity. This point corresponds to the optimum delineating Π value (-0.402). The fractional area under the ROC curve is approximately 0.765, which can be considered analogous to the R-square value of a regression line, confirms the strength of this model.

In Figure 3.8, the bold vertical line at Π=-0.402 is a delineator generated by the ROC curve and which can differentiate poorly absorbed from well-absorbed drugs. In other words, if Π value is greater than -0.402, the compound is likely to be well absorbed, and if Π value is lower than -0.402, the compound is likely to be poorly absorbed. Using horizontal and vertical delineators, this Figure is divided into four quadrants. The 675 points in the upper right (true positive) and 99 points in the lower left (true negative) represent correct predictions of high and low absorption efficiency. The 68 points in the lower right (false positive) and 96 points in upper left (false negative) quadrants represent incorrect predictions.

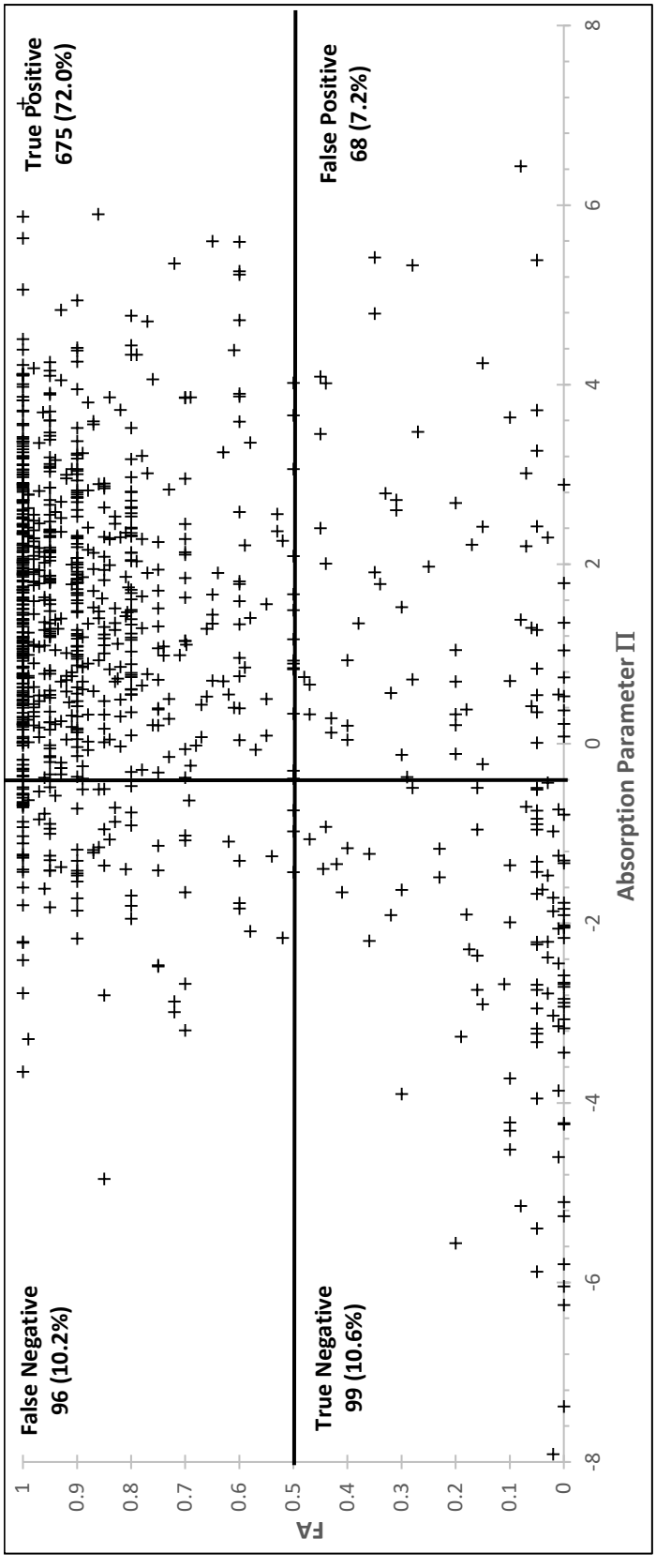

Figure 3.8 Fraction Absorbed vs. Absorption Parameter Π.

For a better understanding of the data in Figure 3.8, the bar graph with standard error is generated by plotting the average of the FA values within -0.5 and +0.5 log units of the Π value. This curve is shown in Figure 3.9. The bar label corresponds to the total number of compounds fall into that Π range. We can observe that Π values and the corresponding mean FA values have a similar trend as we move from negative region to positive region.

Interestingly, a single value of Π (-0.402) is equally applicable to drugs that form solution or suspension in the GI tract. Figure 3.10 represents the drugs that form a solution at their administered dose (Equation 3.8), and Figure 3.11 represents the drugs that form suspension at their administered dose (Equation 3.9). It is clear from these figures and Table 3.1 that a single Π value of -0.402 can differentiate well-absorbed and poorly absorbed compounds for solutions as well as for suspensions.

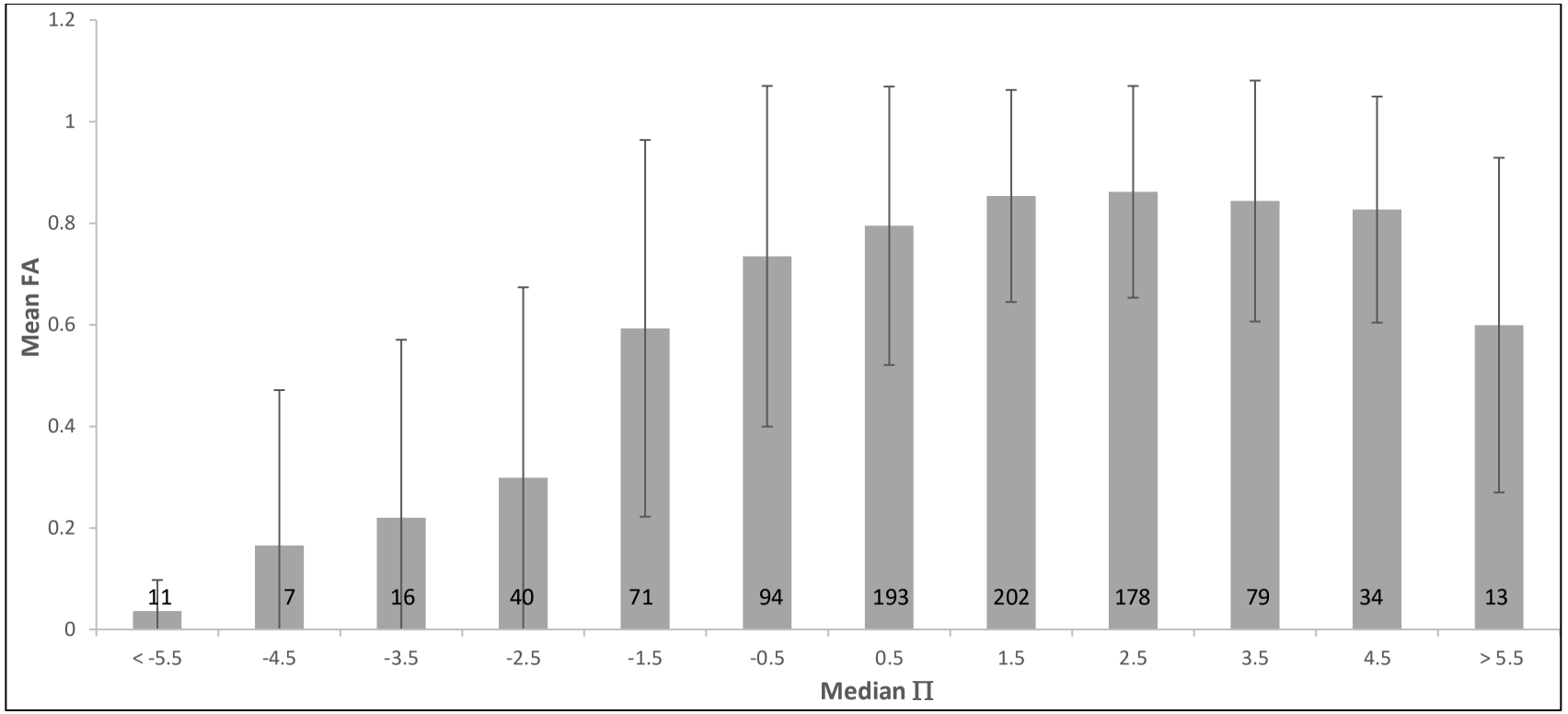

Figure 3.9 The Plot of Mean Fraction Absorbed vs. Median Absorption Parameter Π.

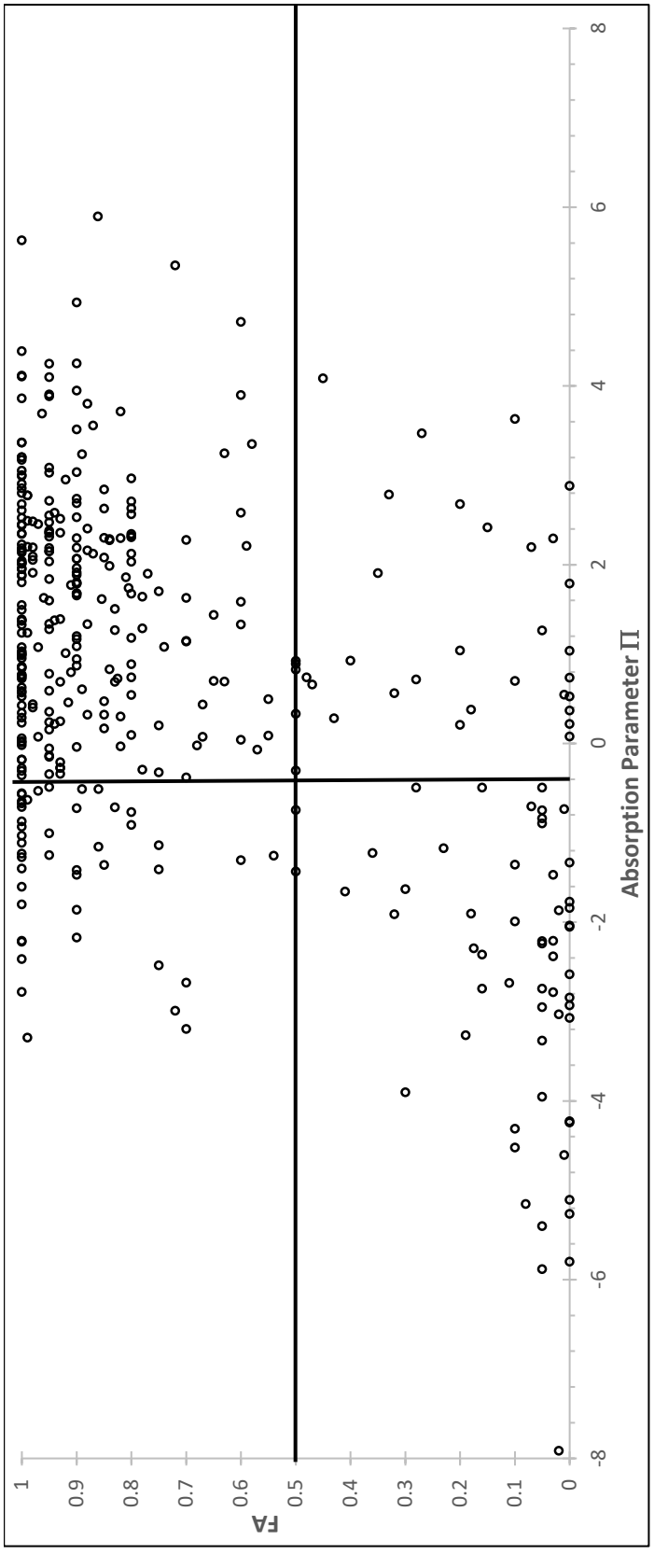

Figure 3.10 Fraction Absorbed vs. Absorption Parameter Π for a Solution.

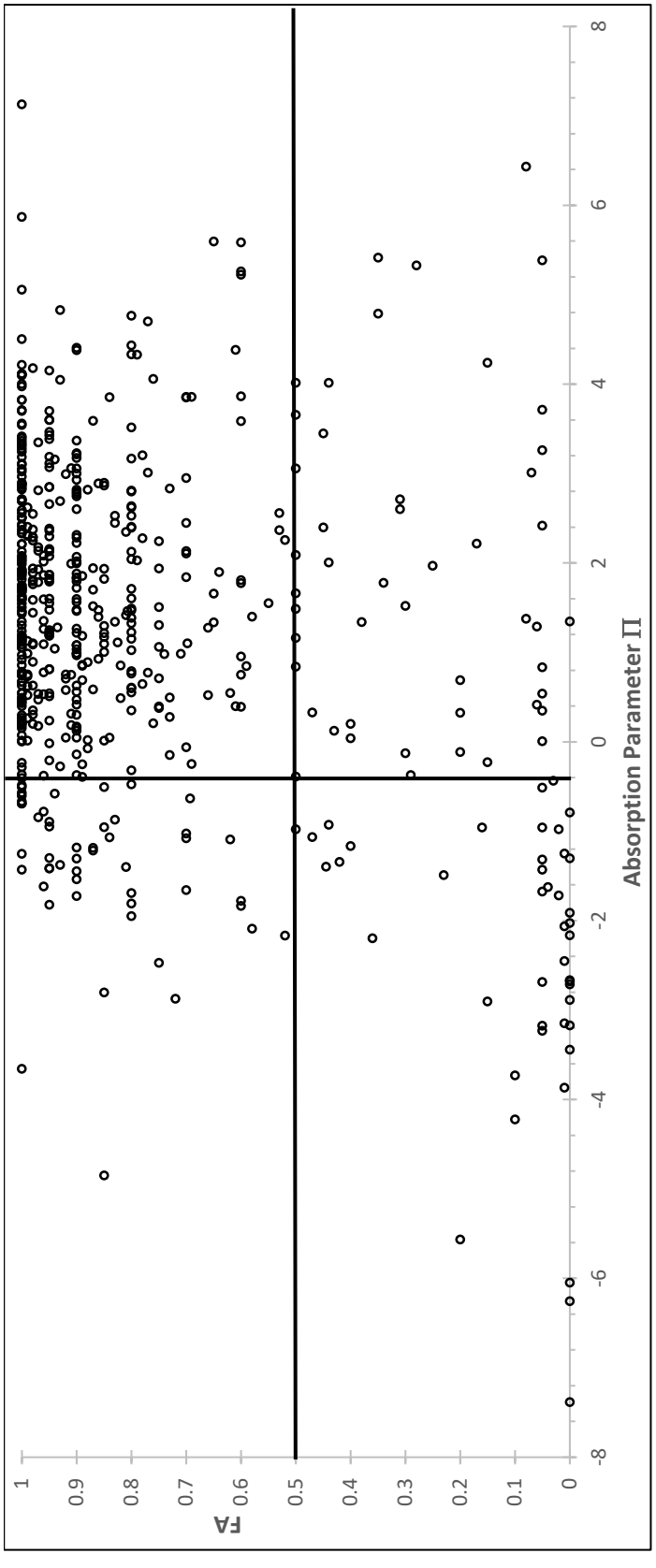

Figure 3.11 Fraction Absorbed vs. Absorption Parameter Π for a Suspension.

Clearly, there is a good correlation between the observed FA and the calculated absorption parameter Π for the whole dataset as well as for 377 drugs that are soluble in 250 ml of GI fluid (solutions) and 561 for immiscible drugs (suspensions). Furthermore, the fraction of the correct predictions is similar for both groups.

Overall, 82.5% of the predictions are correct. The relatively low number of reported poorly absorbed data is partially due to a reluctance of companies to publish negative results.

In 1997, Lipinski *et al.* introduced the rule of five for rapid screening of compounds which has improved bioavailability. According to them, compounds would possess poor absorption if any two of the following conditions met; molecular weight > 500, log K_{ow} >5, the number of hydrogen bond donor >5, the number of hydrogen bond acceptor > 10. To study outliers and whether molecular weight has a significant effect on fraction absorbed or not, a low molecular weight (MW < 150) compounds and high molecular weight (MW > 1000) compounds are plotted in Figure 3.12. It is evident from Figure 3.12 that most of the high molecular weight compounds have a low value of fraction absorbed and most of the low molecular weight compounds have a high value of fraction absorbed. To understand the relationship between molecular weight and fraction absorbed, as showed in Figure 3.13, the plot of mean FA and median molecular weight is generated. It is apparent from this figure that there is no significant change in mean FA value until the molecular weight is 400. However, we can see that increasing molecular weight above 400 will lead to a steady decrease in mean FA value. Camenisch *et al. [59]* observed similar

trend between molecular weight and Caco-2 cell permeability, and Varma *et al.* observed similar trend between molecular weight and bioavailability. [60]

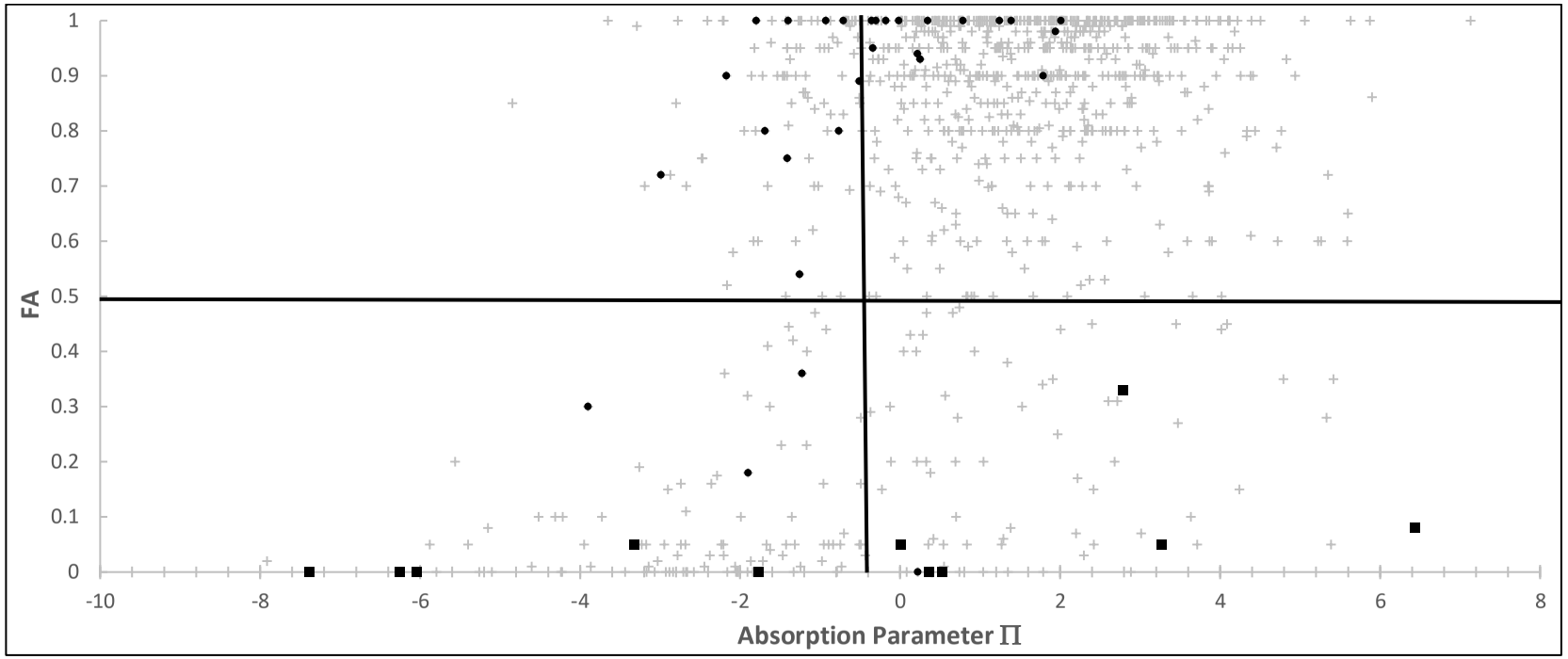

Figure 3.12 Fraction Absorbed vs. Absorption Parameter Π with Low and High Molecular Weight Compounds.

(●) When MW is less than 150 Dalton and (■) When MW is greater than 1000 Dalton

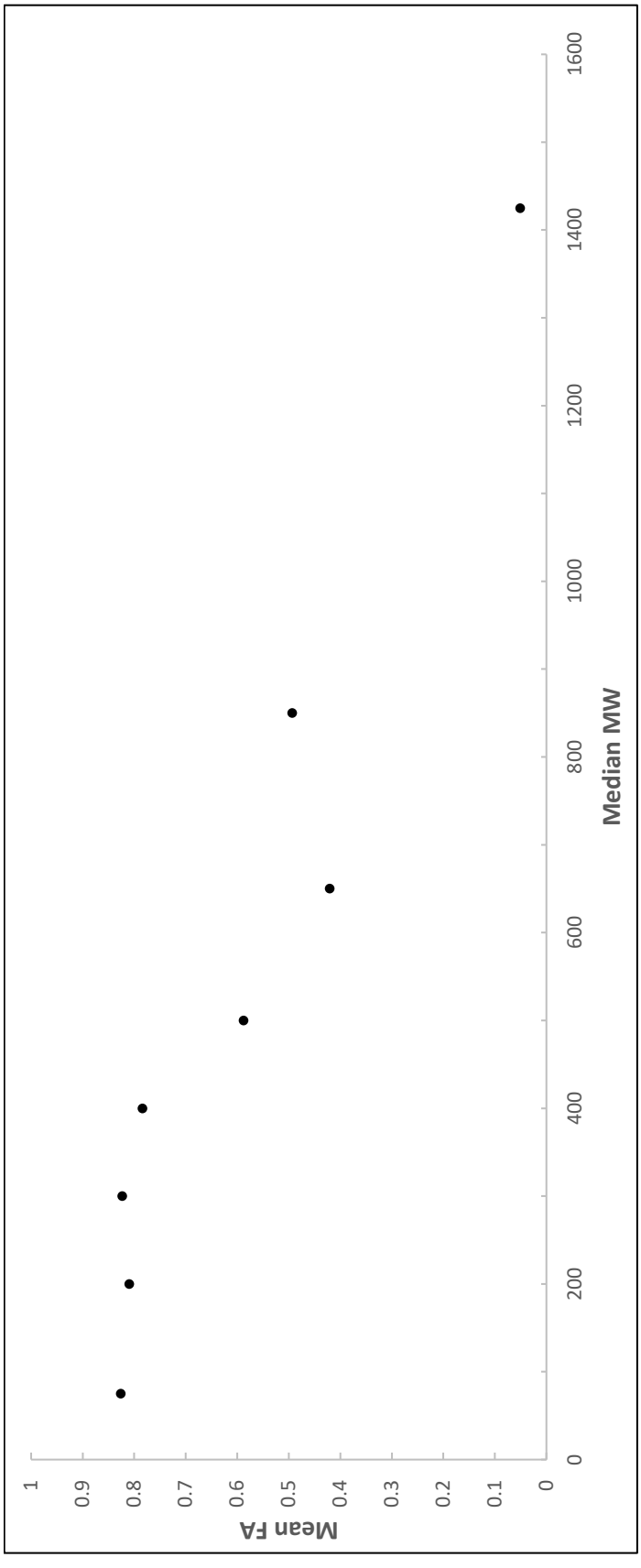

Figure 3.13 The Correlation Between Mean FA and Median MW.

As we discussed earlier, previously reported the rule of unity models were only applied to passively absorbed drugs. For making generalized model, the rule of unity model is applied to all compounds irrespective of their membrane transport mechanisms. In Figure 3.14, the compounds used in this model are divided into three categories; reported to be passively absorbed, reported to have active influx transport, and reported to have active efflux transport. If this model is only applied to passively absorbed compounds, it has overall 84.8 % true prediction power. When this model is applied to all compounds irrespective of their transport mechanism, it still has 82.5 % true prediction power (Table 3.1). It is evident from the overall result that this model can be applied to all compounds irrespective to transport mechanism without losing significant accuracy. Moreover, in very early stage of drug discovery and for virtual compounds, it is hard to get information regarding their membrane transport mechanism. Figure 3.14 shows that out of all false negative outliers, about 23% outliers are reported to have active influx transporter. In other words, based on physicochemical properties as per our model these compounds should be poorly absorbed. However, if active influx transport mechanism is significant, then that can explain why these compounds have higher fraction absorbed value than predicted by our model. Similarly, it is also evident from Figure 3.14 that out of all false positive outliers, about 19% outliers are reported to have active efflux transporter. In other words, based on physicochemical properties as per our model these compounds should be well absorbed, however, if active efflux transport mechanism is significant, it can explain why these compounds have lower fraction absorbed value than predicted by our model.

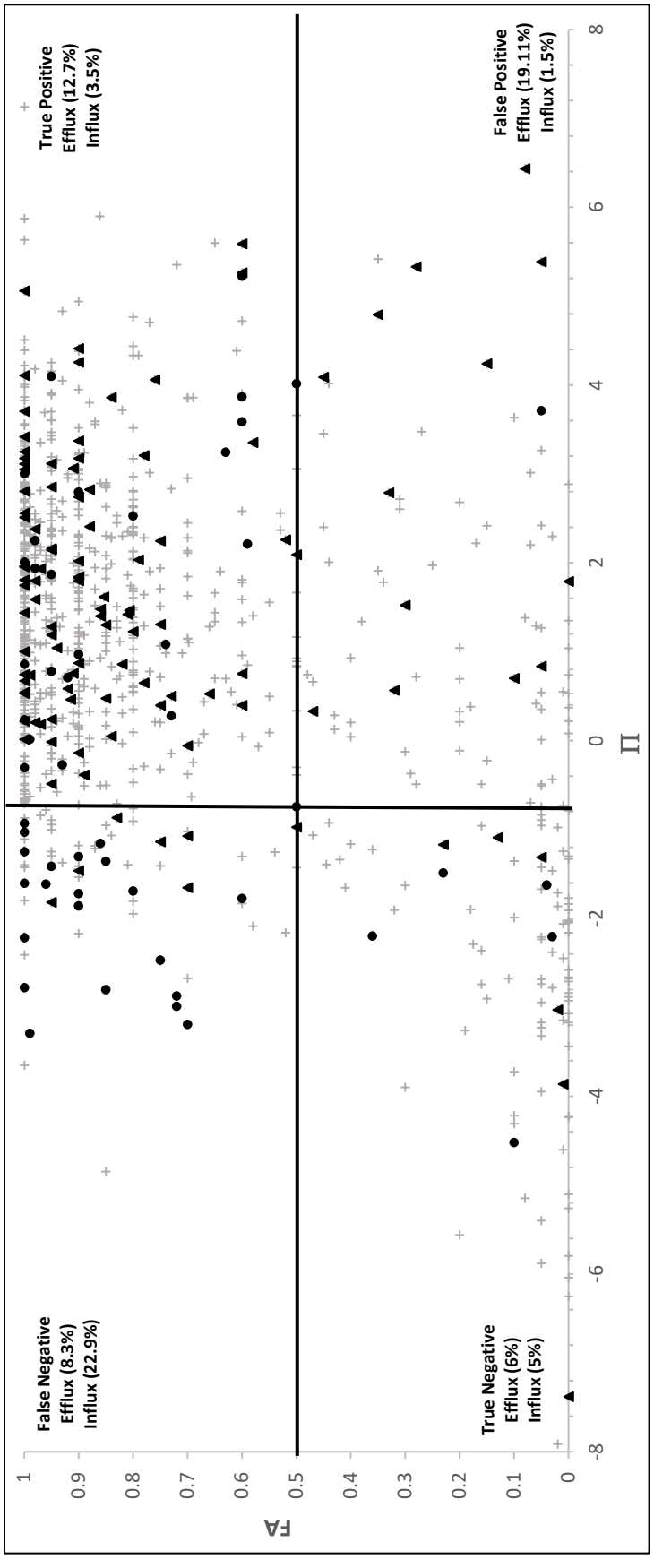

Figure 3.14 Fraction Absorbed vs. Absorption Parameter Π with Absorption Mechanism.

(+) passive transport (●) Influx, (▲) efflux

Since this model is based only on the physical data and dose, it does not account for the physiological conditions of the GI tract or the dissolution kinetics of the drug. Π can be utilized as a pre-screening tool for predicting the absorption efficiency for orally administered drugs. It can also be an aid in the design of drugs for maximum absorption.

Table 3.1 Summary of Predictions for the Pharmaceuticals

Category	Total	True	False	% True
Solutions (4D ≤ Sw)	377	302	75	80.1
Suspensions (4D > Sw)	561	472	89	84.1
Poorly absorbed (FA < 0.5)	167	99	68	59.3
Well-absorbed (FA ≥ 0.5)	771	675	96	87.5
Passive transport	737	625	112	84.8
Active influx	52	29	23	55.7
Active efflux	113	92	21	81.4
All	938	774	164	82.5

3.4 Conclusion

The absorption efficiency of drugs can be characterized based on a single Π value which is a function of the drug dose, and the calculated aqueous solubilities, the calculated octanol-water partition coefficients, and the unitless luminal oversaturation number. If the value of the Π for a drug is greater than -0.402, it is likely to be well (> 50%) absorbed and if Π is less than -0.402, it is likely to be poorly absorbed (< 50%). The reported human intestinal absorption was predicted correctly for 774 out of total 939 compounds considered. Thus, the rule of unity could be utilized as a pre-screening tool in the early stage of drug discovery for predicting absorption for orally administered drugs.

CHAPTER 4

PREDICTION OF MAXIMUM WELL-ABSORBED ORAL DOSE USING THE MELTING POINT

Summary

For an orally administered drug to be bioavailable, it must be efficiently absorbed from the GI tract. In this chapter, the maximum dose that is likely to be well-absorbed upon oral administration is determined using the theoretically derived Π^{MP} absorption model which is based only on the experimental melting point and the dose of drug. Π^{MP} can aid in the early evaluation of drug absorption efficiency. The specific delineator values of $\Pi^{MP} \geq 0$ utilized for calculating maximum well-absorbed dose (fraction absorbed ≥ 0.5).

This human intestinal absorption model is applied to over 500 pharmaceuticals that form saturated solution in the gastrointestinal (GI) tract at the administered dose, and about 84.5% of its predictions are correct. This study will provide a screening tool that can differentiate well-absorbed drugs in the early stage of drug discovery and development. The maximum well-absorbed dose calculated using this model can be utilized as a guideline for preclinical studies.

4.1 Introduction

Predicting human intestinal absorption (HIA) is a challenging task because the absorption of drugs from the gastrointestinal (GI) tract is a complex function of many physicochemical, physiological and pharmaceutical factors. [4] Any model that attempts to account for all these factors will be extremely complicated and not feasible to use in the initial phase of drug discovery. In the proposed simple and intuitive approach, we utilized the melting point and dose of the drug to predict whether the drug is going to be well absorbed (fraction absorbed, FA ≥0.5) or not.

The melting point (MP) is a fundamental physicochemical property of a compound which is mainly used for identification of a compound and as an indication of the compound's purity. Chemists routinely report MP amongst the first experimental properties following the synthesis of a novel material [61]. Numerous models [16-18,62] have been reported in the literature that utilized physicochemical properties to predict absorption potential.

The main objective of this work is to generate the ability to determine whether a specified dose will be well absorbed (fraction absorbed $\geq$ 0.5) on the basis of the experimental melting point value.

4.2 Background

4.2.1 Steady State Membrane Transport Model

In 1972, Stehle and Higuchi [15] developed a new concept of *in vitro* modeling for transport across the membrane. They modified the membrane model by adding poorly stirred aqueous layers adjacent to lipid membrane as additional barriers to transport. Using this model, they showed that transport could be limited by either passage through the membrane or by passage through the aqueous diffusion layers. The transport rate or flux across the membrane (F) is proportional to the product of the drug concentration gradient ($\Delta \mathrm{C}$) and the membrane-water partition coefficient (K_{mw}) of the drug, i.e.,

$$F \propto \Delta \mathrm{C} * \mathrm{K_{mw}} \qquad \text{(Equation 4.1)}$$

Flynn and Yalkowsky [63] showed that the maximum transport rate for a drug across a biological membrane is obtained when the donor solution is saturated with drug concentration and the receptor solution is maintained at near zero concentration, i.e., the concentration gradient of the drug is equal to its intrinsic solubility $\mathrm{S_w^{int}}$. Therefore, the steady state membrane flux from saturated solutions becomes,

$$\mathrm{F}_S \propto \mathrm{S_w^{int}} * \mathrm{K_{ow}} \qquad \text{(Equation 4.2)}$$

where the membrane-water partition coefficient of the drug is assumed to be identical to the octanol-water partition coefficient (K_{ow}).

4.2.2 Absorption Potential Based Models

Dressman *et al.* [16] (1985) proposed an absorption potential ($AP_{Dressman}$) as,

$$AP_{Dressman} = \log\left(\frac{K_{ow} * f_{non} * S_w^{int} * V_L}{D}\right) \quad \text{(Equation 4.3)}$$

where D is the drug dose, K_{ow} is the partition coefficient, S_w^{int} is the intrinsic solubility at 37°C, f_{non} is the fraction in the nonionized form at pH 6.5, and V_L is the intestinal luminal volume.

Balon *et al.* [17] (1999) modified the numerator of the above equation and defined absorption potential (AP_{Balon}) as,

$$AP_{Balon} = \log\left(\frac{S_T^{6.8} * K_D^{6.8} * V_L}{D}\right) \quad \text{(Equation 4.4)}$$

where $S_T^{6.8}$and $K_D^{6.8}$are the total solubility in water and the octanol-water distribution coefficient, respectively, of the drug at pH 6.8.

Assuming a GI luminal volume of 0.250 L, this becomes,

$$\mathrm{AP} = \log\left(\frac{S_T^{6.8} * K_D^{6.8}}{4D}\right) \qquad \text{(Equation 4.5)}$$

4.2.3 Intrinsic Product and its Significance

Shortly thereafter, Ni *et al.* [6] showed that the product of the solubility of a compound in water at any pH (S_T^{pH}) and the octanol-water distribution coefficient at the same pH (K_D^{pH}) is equal to the product of the intrinsic solubility (S_w^{int}) and the intrinsic partition coefficient (K_{ow}^{int}), i.e.,

$$S_T^{pH} * K_D^{pH} = S_w^{int} * K_{ow}^{int} \qquad \text{(Equation 4.6)}$$

This equation is only valid when salt precipitation and ion pair partitioning are insignificant. This relationship holds true for weak acids, weak bases, and zwitterions over a wide pH range. Not only the intrinsic product of a drug is constant, but it also provides a valuable tool for analyzing membrane transport data. Since any change in solubility with pH is accompanied by an equal increase in magnitude and opposite change in Kow, the intrinsic product eliminates the need to know either pKa of the drug or the pH of the biological medium.

Using intrinsic products, Sanghvi *et al.* [18] (2001,2003) modified the absorption potential, and introduced a new absorption parameter ,Π, defined as,

$$\Pi = \log\left(\frac{S_w^{int} * K_{ow}^{int}}{4D}\right) \quad \text{(Equation 4.7)}$$

4.2.4 Dose and Physicochemical Properties Based Models

Both, steady state concept-based AP models and kinetic-based maximum absorbable dose (MAD) models by Johnson and Swindell (1996) [64] and Yu (1999) [65] utilized dose of the drug to predict human intestinal absorption. The drug dose is also important for several drugs classification based on FA, for example, the biopharmaceutics classification system (BCS) by Amidon *et al.* (1995) [66], biopharmaceutics drug disposition classification system (BDDCS) by Wu and Benet (2005) [67], developability classification system (DCS) by Butler and Dressman (2010) [68], dose-dependent biopharmaceutics classification system (DDBCS) by Charkoftaki *et al*. (2012) [69].

4.2.5 Melting Point Based Absorption Potential Model

Earlier, Yalkowsky [7] developed the General Solubility Equation (GSE) which provides a simple means of estimating the intrinsic solubility of a crystalline solute from its octanol-water partition coefficient and melting point.

$$\log(S_w^{int}) = 0.5 - 0.01\,(MP - 25) - \log(K_{ow}^{int}) \quad \text{(Equation 4.8)}$$

or

$$\log(S_w^{int} * K_{ow}^{int}) = 0.75 - 0.01(MP) \quad \text{(Equation 4.9)}$$

where MP is the melting point in degrees Celsius. Note that if the compound is liquid at room temperature, the MP is assumed to be 25°C.

Later, Chu and Yalkowsky [40] combined Equation 4.7 and Equation 4.9 to give the melting point based absorption parameter as

$$\Pi^{MP} = 0.75 - 0.01MP - \log 4D \quad \text{(Equation 4.10)}$$

where Π^{MP} is the Π value calculated using melting point and D is the dose in moles, since it is based on the saturation solubility, this equation also reflects the maximum flux across the membrane solely as a function of melting point and drug dose.

In 1986, Schultz and Ando [70] developed a model that showed direct correlation between lipid membrane diffusional transport and lipophilic-eutectic parameter (L_e). Their calculation is based on the lowering of the melting point of the pure compound by making the eutectic mixture with structurally similar impurity. They observed that intestinal absorption in rats and transdermal absorption in humans show excellent correlation with respect to increasing L_e (or lowering MP of pure compound).

4.2.6 Maximum Well-Absorbed Dose

Previously, Sanghvi *et al.* [18,19], Chu and Yalkowsky [40], Yalkowsky *et al.* [37], and Patel *et al.* [71,72] showed that when Π is greater than or equal to zero, the drug is likely to be well absorbed (FA ≥0.5). Thus, maximum well absorbable dose for saturated solutions is,

$$0.75 - 0.01MP - \log 4D \geq 0 \qquad \text{(Equation 4.11)}$$

or

$$D \leq \frac{10^{0.75 - 0.01MP}}{4} \qquad \text{(Equation 4.12)}$$

According to Equation 4.12, when dose (in moles) is less than or equal to the right side of the equation, the dose is likely to be well absorbed (FA ≥0.5).

4.3 Method

4.3.1 Compound Selection

The previous models [18,19,37,40,71,72] were only applied to nonelectrolyte drugs which were reported to be passively absorbed after oral administration. To make a more robust and a more generalized model, we have incorporated many types of pharmaceuticals including salts, nonelectrolytes, as well as the drug that forms solution or suspension at a given dose, or the drug that are reported to undergo active influx or efflux transport. The compounds which do not follow the GSE assumptions were removed from the overall database.

4.3.2 Fraction Absorbed Data

Most of the experimental FA values were obtained from Hou *et al.* [38] and Newby *et al.* [39] When more than one value was reported, or the value was reported as a range, the mean value was used in this database. The fraction absorbed data are given in supplementary information Table A.2 along with the physical property data and the Maximum Recommended Therapeutic Dose (MRTD) values for each compound. It is noted that the reported FA values are skewed towards well-absorbed values largely because poorly absorbed results are often not reported in the literature.

4.3.3 Log K_{ow}

To eliminate any bias, all log K_{ow} values were collected from chemical abstract service – SciFinder [55] which were calculated using ACDLABS 11.02 software. If values were not available in SciFinder, then ACDLAB 7.0 [57] software was used to calculate all physicochemical properties.

4.3.4 Drug Dose Data

The FDA's MRTD database [41] was chosen to collect most of the drug doses because most of its values were determined from the results of pharmaceutical clinical trials. Values in this database are normalized for the average 60 kg adult. If the dose was not available in the database, then the dose listed in Micromedex [42], Lexicomp [43], or Newby *et al.* [39] was used. This database contains widely distributed doses, and there is no single delineator that can differentiate well-absorbed and poorly-absorbed compounds solely based on their dose value.

4.3.5 Melting Points

Most of the melting points for this study were collected from either the Merck Index [73], companies chemical catalogs, or the scientific literature. [74-239] The melting point values and references are given in supplementary material in Table A.2. If the experimental melting point is not available, then the decomposition temperature is used.

If the drug is marketed as a salt form, the melting point of its corresponding nonelectrolyte is used. If the experimental melting point is not available, then group contribution methods like UPPER can be utilized to calculate theoretical melting point (Chapter 5). The lack of correlation between the experimental FA value and the experimental melting point is shown in Figure 4.1.

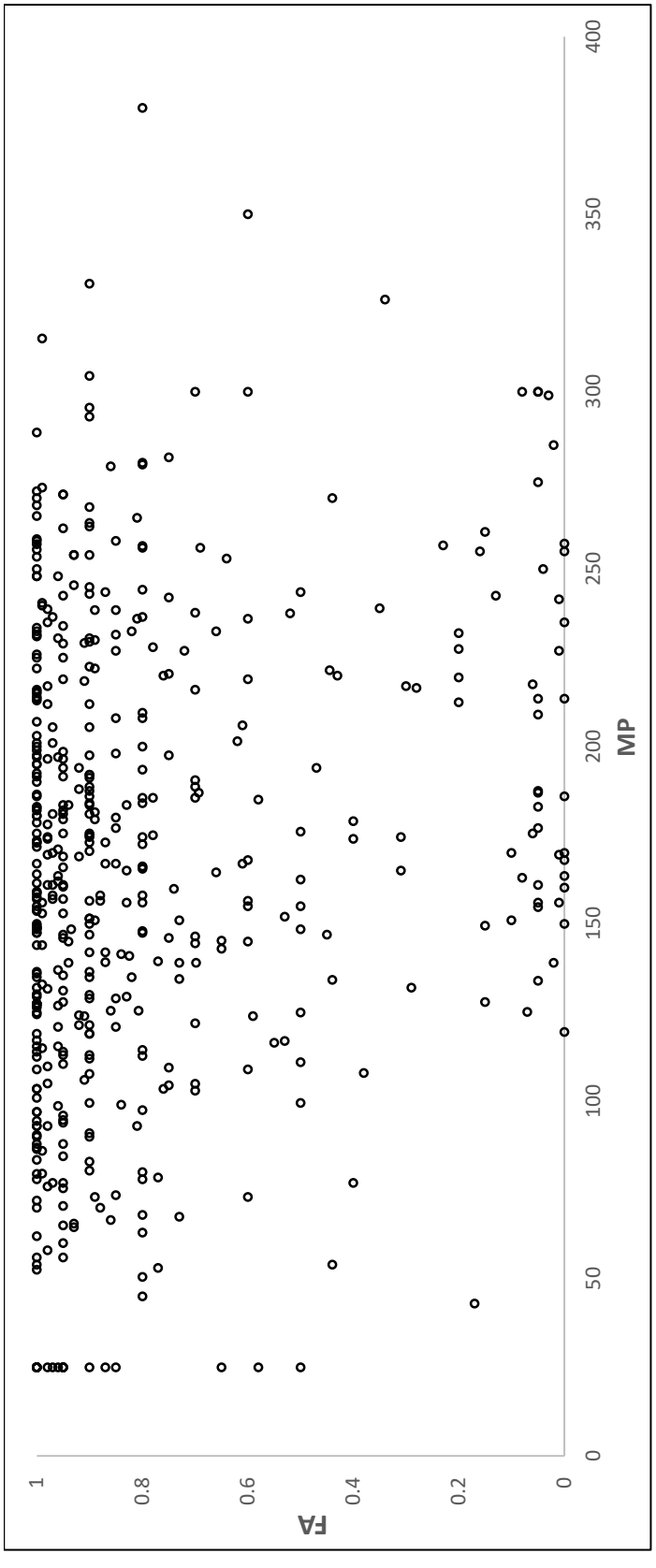

Figure 4.1 The Correlation Between the Fraction Absorbed vs. Melting Point.

4.4 Results and Discussion

According to Equation 4.10, both melting point and drug dose are important for calculating the melting point based absorption parameter (Π^{MP}) The correlation between Π^{MP} and experimental FA for all drugs in suspension is shown in Figure 4.2. The horizontal line at FA=0.5 differentiates the well-absorbed (FA≥0.5) and poorly absorbed (FA<0.5) compounds. The vertical line at Π^{MP} =0 is a delineator corresponding to Equation 4.11 which can differentiate poorly absorbed and well- absorbed drugs.

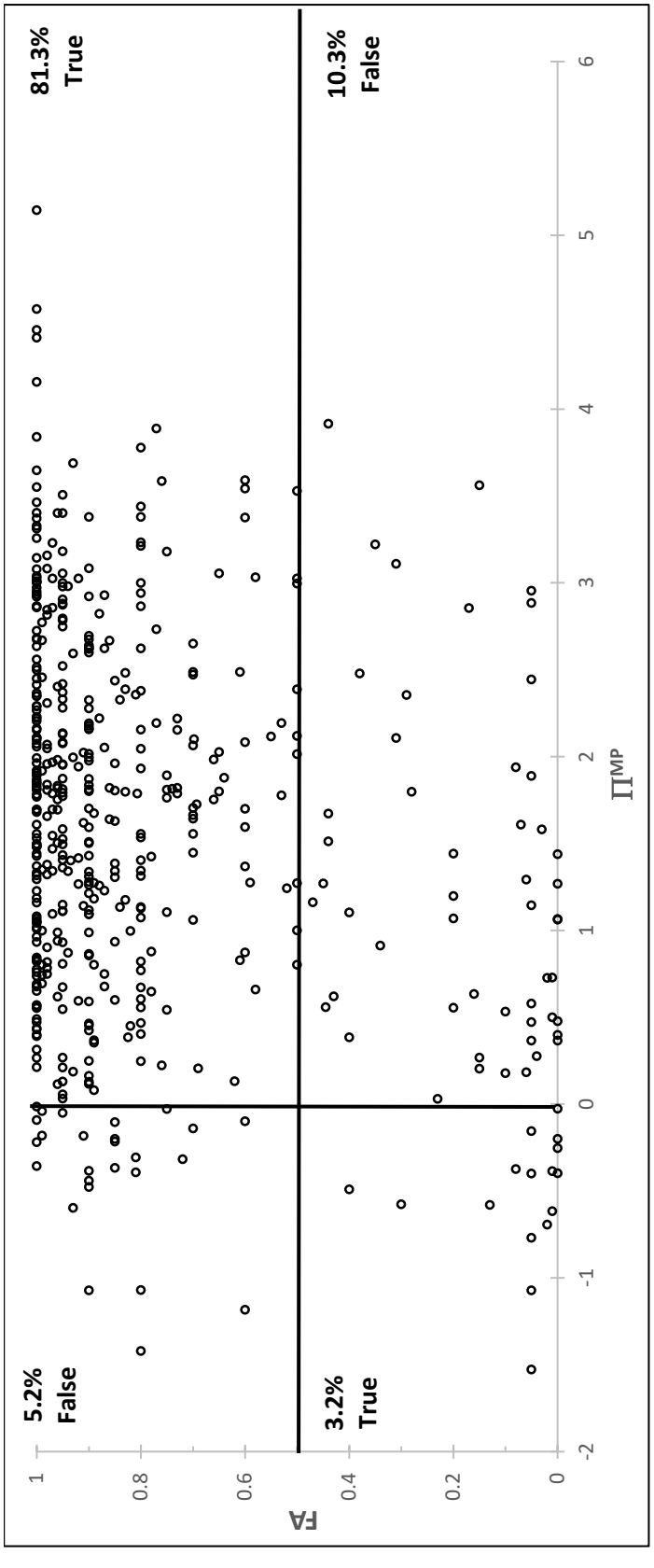

Figure 4.2 Fraction Absorbed vs. Absorption Parameter Π^{MP} for Suspensions.

In other words, if a Π^{MP} value is greater than zero, the compound is likely to be well absorbed. This Figure is divided into four quadrants. The 408 points in the upper right and 16 points in lower left represent correct predictions. The 52 points in the lower right and 26 points in upper left quadrants represent incorrect predictions.

It is worth noting that the derivation of Π^{MP} is based on the solubility product, which is applicable for drug concentrations that exceed their solubilities. However, in the early stage of drug design and development, neither the drug dose or its solubility are known. Fortunately, we have empirically observed that the application of Π^{MP}, by Equation 4.12, to all compounds, without regard to whether they form solutions or suspensions in the gut (See Figure 4.3) gives similar results to those for suspensions (See Figure 4.2). Therefore, Equation 4.12 can be used to calculate the maximum well absorbable dose.

This dose for 820 compounds is recorded in supplementary information in Table A.1. According to our results, overall 83% of the calculated maximum well-absorbed dose is correct. The relatively low number compounds in the lower left quadrant may be due to a reluctance of scientists, companies, and journals to publish negative results.

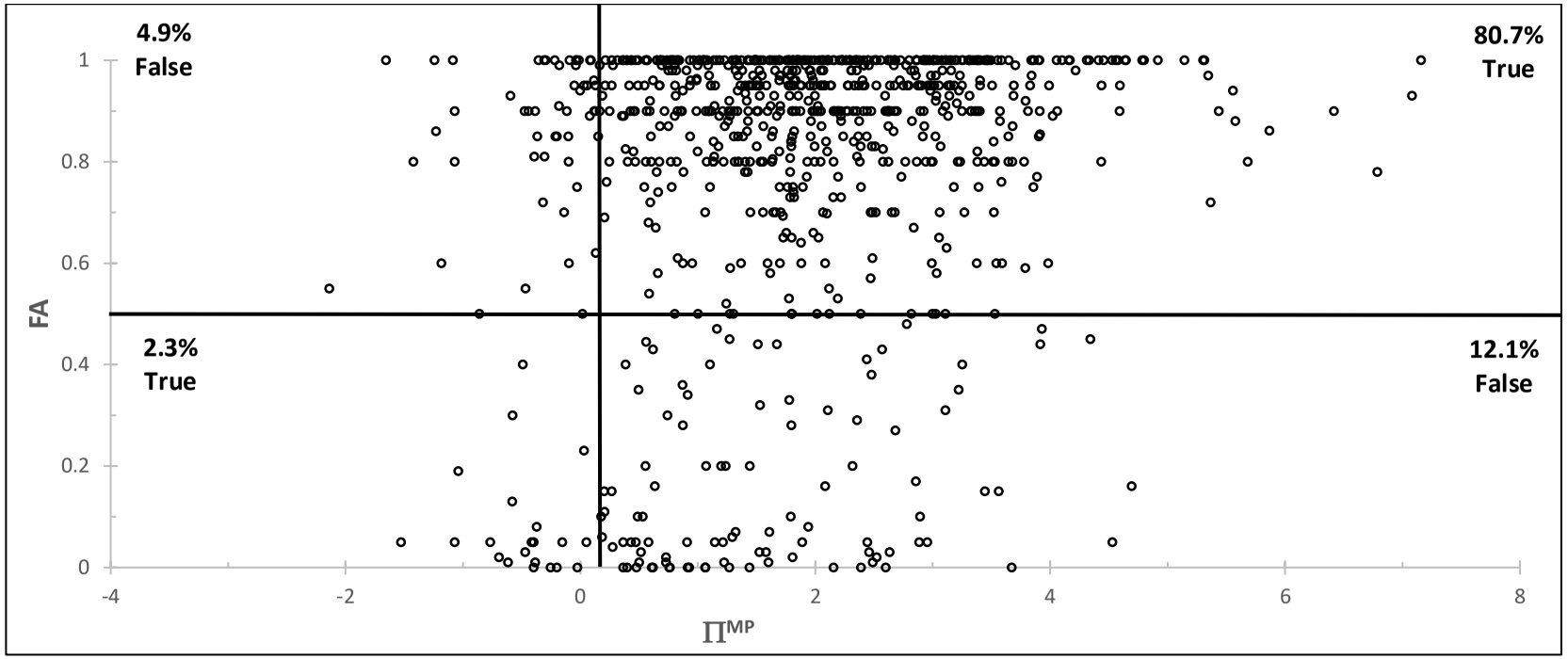

Figure 4.3 Fraction Absorbed vs. Absorption Parameter Π^{MP} for All Pharmaceuticals.

Clearly, there is a correlation between the value of the fraction absorbed and Π^{MP}, however, It is difficult to generate a single equation that can predict the relationship between FA and Π^{MP}. For a better understanding of these data, the bar graph with standard errors is generated by plotting the average of the FA values within -0.5 and +0.5 log units of the Π^{MP} value. This curve is shown in Figure 4.4. In the left region, standard errors are large compared to the right regions. The bar label corresponds to the number of compounds that fall into that Π^{MP} range. We can observe a sharp drop in Mean FA value between the Π^{MP} value of -0.5 and +0.5.

Using over 300 compounds, Newby *et al.* [39] also demonstrated that the model based on Π^{MP} and the GSE solubility has higher accuracy than using experimental solubility, and it can be utilized to predict oral absorption. Recently, Duosani and Macheras [240] showed that how simple absorption parameter Π can be utilized to understand complicated homogeneous and heterogeneous aspects of drug absorption kinetics.

For a better understanding and to see the overall trend, mathematical treatment is performed on the whole dataset. Table 4.1 shows the relationship of average melting points to various mean properties used in this model. The mean properties calculated based on 820 compounds are listed in Table 4.1.

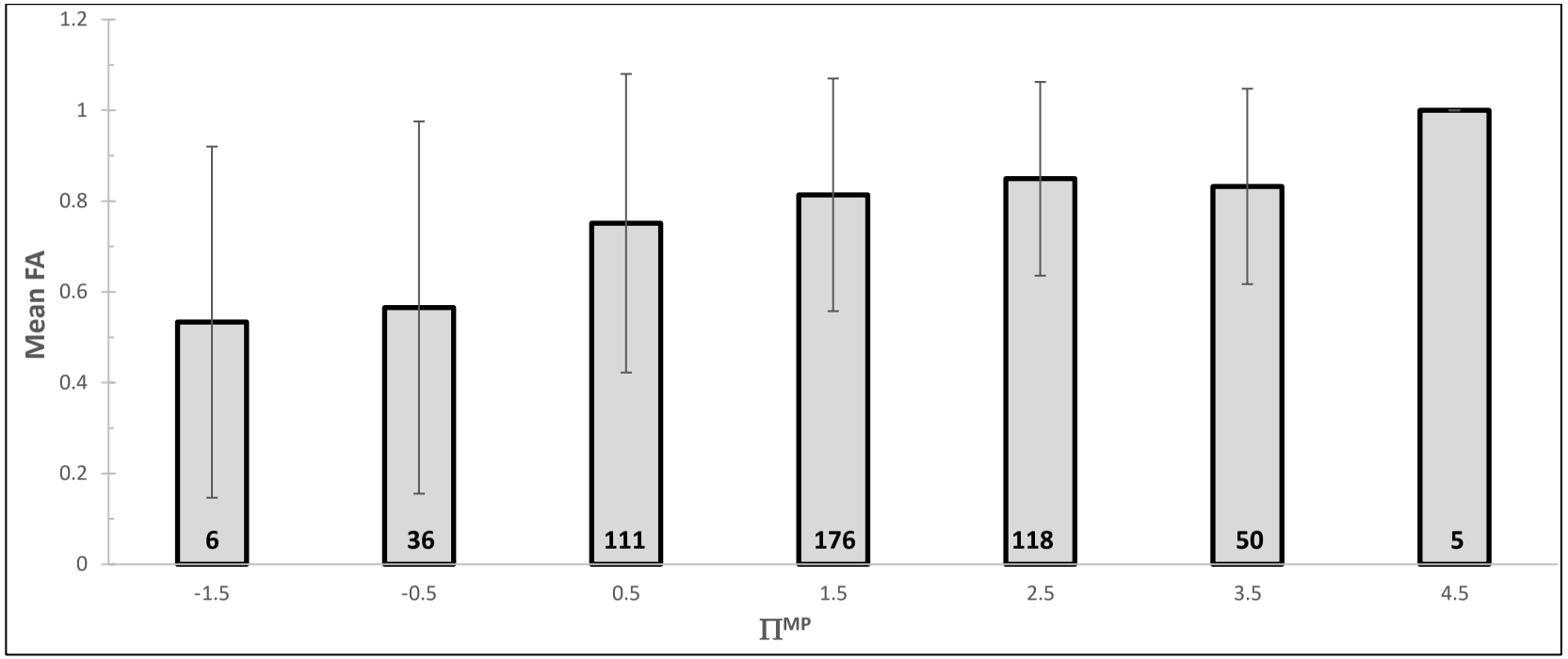

Figure 4.4 Mean Fraction absorbed vs. Median Π^{MP} Along with the Standard Error.

Table 4.1. The Interrelationships Among Mean MP, Mean log 4D, Mean FA, and Mean Π^{MP}

Melting point range	Total number of compounds	Mean value			
		MP	log 4D	FA	Π^{MP}
Below 50	24	27	-2.42	0.88	2.90
50 - 100	63	78	-2.41	0.90	2.38
100 - 150	118	129	-2.54	0.82	2.00
150 - 200	154	174	-2.43	0.78	1.44
200 - 250	91	226	-2.59	0.74	1.07
250 - 300	46	270	-2.37	0.68	0.41
Above 300	6	334	-2.02	0.76	-0.57

This model is based only on the experimental melting point and the dose; it does not account for the physiological conditions of the GI tract or the dissolution kinetics of the drug. This simple absorption parameter Π^{MP} can be utilized as an early screening tool for predicting the maximum well-absorbed dose. It can also be an aid in drug design to synthesize drugs which have high oral absorption potential.

4.5 Conclusion

The simple and intuitive absorption parameter Π^{MP} is a function of the drug dose and experimental melting point. If the value of the Π^{MP} for the orally administered drug is greater than zero, it is likely to be well (> 50%) absorbed. The maximum well-absorbed dose was predicted correctly for 424 out of total 502 drugs that form a saturated solution in the gastrointestinal tract (GI) at the administered dose. Interestingly, both experimental mean FA and calculated Π^{MP} show a similar trend with an increase in mean MP. Therefore, the absorption parameter Π^{MP} could be utilized as a pre-screening tool in the early stage of drug discovery. The maximum well absorbable dose calculated using this model can guide preclinical studies.

CHAPTER 5

PREDICTION OF MELTING POINT AND AQUEOUS SOLUBILITY OF BARBITURATES

Summary

Classical barbiturates are formed by substituting one or both hydrogen atoms at the 5-position with alkyl, aryl, and/or alicyclic groups. In this study, a previously developed UPPER (**U**nified **P**hysicochemical **P**roperty **E**stimation **R**elationships) approach is applied to predict the melting points and aqueous solubilities of a series of barbiturates. The descriptors from a previously developed UPPER model on hydrocarbons are used to generate new descriptors for the barbiturate ring using multiple linear regression analysis. Melting points can be predicted solely from additive enthalpic and non-additive entropic descriptors. These predicted melting points and aqueous activity coefficients are used to predict the aqueous solubilities. Only three new parameters are added to predict the each of above properties. The average absolute errors in the prediction of melting points and aqueous solubilities are 20.6^{o}C and 0.57 respectively. This simple and efficient UPPER approach can be useful for predicting melting points and aqueous solubilities of novel barbiturates and other compounds for which the experimental values are unavailable in the literature. The UPPER based solubility and melting point can be utilized for calculating maximum well-absorbed dose for virtual compounds.

5.1 Introduction

Classical barbiturates are malonyl urea derivatives substituted at the five position with alkyl, aryl and/or alicyclic groups [241] (Figure 5.1). Since the introduction of barbiturates by Baeyer in 1864, more than 2500 derivatives have been synthesized, and a few of them are still being marketed [242]. The present work focuses on predicting the melting points and aqueous solubilities of the classical barbiturates from their chemical structures.

Drug discovery is a very expensive and difficult process. In order to minimize the overall cost and speedup the process, many approaches have been developed to estimate physicochemical properties of drugs before they are synthesized [40,243]. The UPPER approach developed by Yalkowsky *et al.* [244] offers a rapid and inexpensive means of calculating melting points, vapor pressures, aqueous solubilities and other biorelevant properties.

The melting point has wide application in the field of pharmaceutical, biochemical and environmental sciences because of its relationship with the solubility and vapor pressure [245]. Recently, Lian *et al.* used the UPPER model for predicting the melting point of hydrocarbons [246].

The aqueous solubility is an important determinant of dissolution rate, absorption, and bioavailability. Poor aqueous solubility is a key problem during formulation development and drug design [247]. The GSE (General Solubility Equation) developed by Jain and

Yalkowsky requires the calculated octanol-water partition coefficient and the experimental melting point to predict the aqueous solubility [7]. Yalkowsky and Pinal used the GSE to calculate the aqueous solubility of several barbiturates [248].

In this chapter, we applied the UPPER model only to the classical barbiturates. As in these type of barbiturates, the general ring structure has only other substitution at five position is hydrocarbon moieties (Figure 5.1). Here, only UPPER model is used to predict the melting points while both UPPER and GSE models are used to calculate the aqueous solubilities of barbituric acid derivatives.

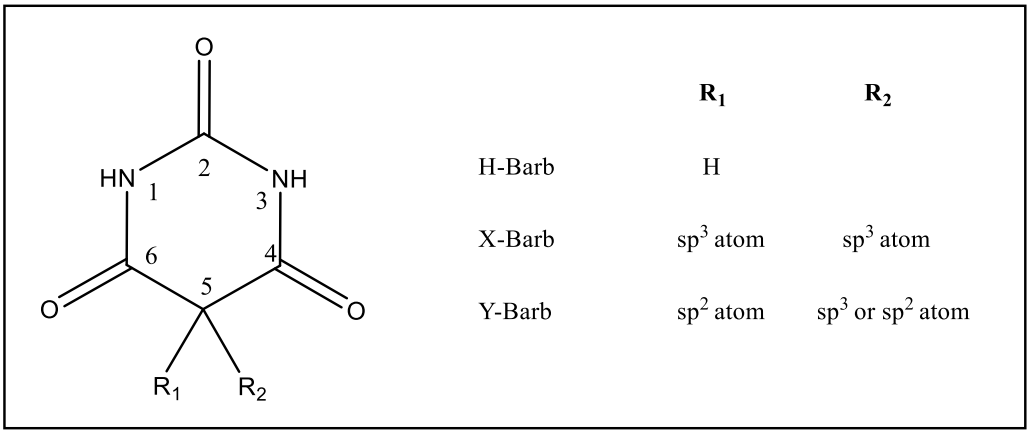

Figure 5.1 General Structure of Barbiturates (R_1, R_2 = H, alkyl, aryl, and/or alicyclic).

5.2 The UPPER Model for Melting Point Prediction

Melting points T_m (K) are calculated using Equation 5.1.

$$T_m = \frac{\Delta H_m}{\Delta S_m} \quad \text{(Equation 5.1)}$$

where ΔH_m is the total enthalpy of melting (kJ/mol), and ΔS_m is the total entropy of melting (J/K · mol) as described below.

5.2.1 Enthalpy of Melting

The enthalpy of melting is defined as the total change in the enthalpy when one mole of a crystal is converted into a liquid. i.e.,

$$\Delta H_m = H^L - H^C \quad \text{(Equation 5.2)}$$

where H^L is the molar enthalpy of a liquid phase and H^c is the molar enthalpy of a crystal phase.

The enthalpy of melting is an additive property that can be calculated by the sum of constituent group contributions as expressed in Equation 5.3.

$$\Delta H_m = \sum n_i m_i \quad \text{(Equation 5.3)}$$

where n_i is the number of times that group i appears in the compound, and m_i is the contribution of group i to the total enthalpy of melting.

5.2.2 Entropy of Melting

The entropy of melting is defined as the change in the molar entropy when the crystal is converted into a liquid phase. Hence,

$$\Delta S_m = S^L - S^C \qquad \text{(Equation 5.4)}$$

where S^L is the molar entropy of a liquid phase and S^c is the molar entropy of a crystal phase. Based on the Boltzmann equation, the molar entropy of melting is related to the logarithm of ρ_m, the ratio of the probabilities of existence of the crystal phase to that of the liquid phase. That is

$$\Delta S_m = -R \ln \rho_m \qquad \text{(Equation 5.5)}$$

where

$$\rho_m = \frac{P^C}{P^L} \qquad \text{(Equation 5.6)}$$

where P^C and P^L are the probabilities of achieving the crystal and liquid state, respectively.

The probability of achieving the crystal phase is equal to the number of ways in one mole of molecules can be arranged that conform to the requirements of a crystal, divided by the total number of ways in which all possible phases can exist. In the case of a substance that exists only as a liquid and a solid phase,

$$P^C = \frac{\Omega^C}{(\Omega^C+\Omega^L)} \text{ and } P^L = \frac{\Omega^L}{(\Omega^C+\Omega^L)} \qquad \text{(Equation 5.7)}$$

where the numerators are the number of ways in which the crystal and liquid can be achieved, respectively and the denominator is the total number of ways in which the molecule can exist.

Combining Equations 5.4 thru 5.7 gives,

$$S^C = -R\ln\frac{\Omega^C}{(\Omega^C+\Omega^L)} \text{ and } S^L = -R\ln\frac{\Omega^L}{(\Omega^C+\Omega^L)} \qquad \text{(Equation 5.8)}$$

where R is the gas constant.

Walden [12] estimated the entropy of melting of a variety of coal tar derivatives as approximately 57 J/K·mol (Walden's Rule). This constant value of the entropy of melting is traditionally used for all organic compounds. However, deviations from Walden's rule are common.

Bondi reported that the total entropy of melting could be explained as the sum of its rotational (ΔS_m^{rot}), conformational (ΔS_m^{conf}) and expansional (ΔS_m^{expan}) components [249].

$$\Delta S_m = \Delta S_m^{rot} + \Delta S_m^{conf} + \Delta S_m^{expan} \quad \text{(Equation 5.9)}$$

Three geometric descriptors; symmetry (σ), flexibility (ϕ) and eccentricity (ε) are used in UPPER to characterize each type of entropic component, respectively.

5.2.2.1 Rotational symmetry

As described by Lian and Yalkowsky, the rotational symmetry (σ) is defined as the number of positions into which a molecule can be placed that are identical to a reference position [246]. Since highly symmetrical molecules can crystallize more readily, they have lower entropies of melting. If the rotational symmetry number is incorporated as the probability ratio into the Boltzmann equation (Equation 5.5), then

$$\Delta S_m^{rot} = -R \ln \sigma \quad \text{(Equation 5.10)}$$

5.2.2.2 Molecular flexibility

The molecular flexibility number (ϕ) is related to the ratio of the total number of possible conformations of a compound in the crystal to that of the liquid. The conformational

component of entropy is related to the molecular flexibility as highly flexible molecules can have many conformations in the liquid and are less likely to be in the single trans conformation of crystal. Thus, they tend to have higher entropies of melting. By incorporating the flexibility number as the probability ratio into the Boltzmann equation, we get

$$\Delta S_m^{rot} = -R \ln \phi \qquad \text{(Equation 5.11)}$$

For a hypothetical long chain normal alkane with completely free bond rotation (assuming equal energies for the trans and two gauche conformations), the probability of being in the all-trans form would be 0.33. According to Wunderlich [250], the trans conformation is more stable than the gauche conformation by 2.09 KJ/mol, and certain combinations of adjacent gauche conformations would place two atoms in the same place. Correcting for these effects gives the overall probability of a molecule being in the all trans form is

$$\phi = (0.4)^{\Phi} \qquad \text{(Equation 5.12)}$$

where Φ, the effective number of torsional units in the molecule.

In UPPER, this effective number of torsional units is calculated using Equation 5.13.

$$\Phi = \text{LIN} + 0.3\ \text{ROT}^* + 0.5(\text{BR} + \text{SP2} + \text{RING}) - 1 \qquad \text{(Equation 5.13)}$$

where LIN is the sum of all non-ring, non-terminal sp^3 atoms; ROT* is the sum of all freely rotating linear chain sp^3 atoms less 4 (e.g. Octane has six linear chain sp^3 atoms, so ROT* value is 2); BR is the sum of all branched, non-ring sp^3 atoms; SP2 is the sum of all non-ring, non-terminal sp^2 atoms; RING is the total number of independent single, fused or conjugated aromatic rings present in the molecule.

5.2.2.3 Molecular eccentricity

Molecular eccentricity (ε) is defined as the total number of atoms in the aromatic and/or aliphatic rings. It is related to the packing efficiency of molecules in the crystal, and thus, to the amount of expansion required for melting. Since highly eccentric molecules are more likely to pack efficiently in the crystal, they need more expansion to from a liquid. This gives them a higher entropy of melting. By substituting the probability ratio of the Boltzmann equation with the eccentricity, we get

$$\Delta S_m^{expan} = R\ ln\ \varepsilon \qquad \text{(Equation 5.14)}$$

Using Equation 5.9, 5.10, 5.11, and 5.14, the total entropy of melting can be described as

$$\Delta S_m = W' - R \ln \sigma - R \ln \phi + R \ln \varepsilon \qquad \text{(Equation 5.15)}$$

where W' is the modified Walden's Rule constant.

In base 10 logarithmic terms it can be represented as,

$$\Delta S_m = W' - 19.1 \log \sigma + 7.6\ \Phi + 19.1 \log \varepsilon \qquad \text{(Equation 5.16)}$$

As described by Lian and Yalkowsky [246], deviation from ideal entropy of melting is common, the entropy of melting for hydrocarbons can be well described by the following empirical equation

$$\Delta S_m = 43.54 - 8.95 \log \sigma + 7.93\ \Phi + 9.16 \log \varepsilon_{ar} + 9.43 \log \varepsilon_{al} \qquad \text{Equation 5.17)}$$

where ε_{ar} and ε_{al} are the molecular eccentricity contribution for the aromatic and the aliphatic rings respectively.

The lower coefficients in Equation 5.17 reflect the fact that the crystal is not a perfect crystal and the liquid is not a perfect liquid.

5.3 The UPPER Model for Intrinsic Solubility Prediction

5.3.1 Ideal Solubility

The ideal solubility of a crystalline solute, X_i^C, is its solubility in a hypothetical perfect solvent, i.e., one in which the solute-solvent interactions are exactly equal to the sum of the solute-solute and solvent-solvent interactions. It is entirely dependent on the crystallinity of the solute and independent of the solvent. The ideal solubility can be

thought of as the ratio of the solubility of a crystal in any solvent to the solubility of its hypothetical supercooled liquid in the same solvent. The ideal solubility is approximated from the Clausius-Clapeyron equation or the Van't Hoff equation, both of which can be expressed as Equation 5.18 [7],

$$logX_i^C = -\Delta S_m \frac{(T_m - T)}{2.303\ R\ T} \quad \text{(Equation 5.18)}$$

where T and T_m are the room temperature and melting point in Kelvin, and R is the gas constant.

5.3.2 Approximate Ideal Solubility

Incorporating Walden's Rule (ΔS_m=57 J/K mol) into the above equation gives,

$$logX_i^C = -0.01\ (T_m - T) \quad \text{(Equation 5.19)}$$

which can be written in Celsius as,

$$logX_i^C = -0.01\ (MP - 25) \quad \text{(Equation 5.20)}$$

5.3.3 Aqueous Activity Coefficient

The logarithm of the aqueous activity coefficient log γ_w (like the enthalpy of melting) is a group additive property. Myrdal and Yalkowsky developed the AQUAFAC (AQUeous Functional group Activity Coefficients) model to calculate the total logarithmic aqueous activity coefficient by adding all group contribution as expressed in Equation 5.21 [251].

$$\log \gamma_w = \sum n_i q_i \qquad \text{(Equation 5.21)}$$

where n_i is the number of times that group i appears in a compound and q_i is the contribution of group i to the total logarithmic aqueous activity coefficient.

5.3.4 Aqueous Solubility

The molar aqueous solubility (S_w) is the ratio of the ideal solubility of a solute to its aqueous activity coefficient [252]. In logarithmic terms it is,

$$\log S_w = log\ X_i^c - log\ \gamma_w \qquad \text{(Equation 5.22)}$$

where $log\ X_i^c$ is obtained by Equation 5.18 and $log\ \gamma_w$ by Equation 5.21.

5.4 Experimental

5.4.1 Data collection

The reported experimental melting point and aqueous intrinsic solubility values of 44 5-substituted barbiturates were collected from Prankerd and McKeown [253], Pinal and Yalkowsky [248], Hughes *et al.* [254], and the Merck Index [11] are listed in Table 5.1. This table includes the melting points (which range between 364 K to 561 K) and aqueous molar intrinsic solubilities (which range between 3.45 E-5 M to 0.12 M). The partition coefficient (log P) values were obtained from Advanced Chemistry Development Software V11.02 [255].

Table 5.1. Experimental and Predicted Melting Point and Aqueous Solubility

No	Name of Barbiturate	Exp. MP (K)	Pred. MP (K)	Residual	Exp. log S_w	GSE log S_w	Residual	UPPER log S_w	Residual
1	5,5-Diethylbarbiturate	463	431	32	-1.40	-1.95	-0.56	-1.47	-0.07
2	5,5-Di-i-propylbarbiturate	501	505	4	-2.77	-3.04	-0.27	-2.41	0.36
3	5,5-Dimethylbarbiturate	551	482	69	-1.74	-1.82	-0.07	-0.26	1.48
4	5,5-Diphenylbarbiturate	561	539	22	-4.20	-2.38	1.81	-3.18	1.02
5	5,5-Dipropylbarbiturate	420	392	27	-2.47	-2.54	-0.07	-2.46	0.01
6	5-Allyl-5-neopentylbarbituric acid	429	426	3	-2.80[p]	-3.01	-0.22	-2.50	0.30
7	5-Allyl-5-phenylbarbiturate	432	436	4	-2.37	-1.84	0.53	-1.70	0.67
8	5-Ethyl-5-(1-ethylbutyl) barbituric acid	395	400	5	-3.06[p]	-3.16	-0.10	-3.51	-0.45

9	5-Ethyl-5-(3-methylbut-2-enyl) barbiturate	431	441	9	-2.25	-2.69	-0.44	-2.18	0.07
10	5-Ethyl-5-allylbarbiturate	435	415	20	-1.61	-1.80	-0.18	-1.02	0.59
11	5-Ethyl-5-heptylbarbiturate	391	391	0	-3.22	-3.78	-0.56	-4.42	-1.20
12	5-Ethyl-5-nonylbarbiturate	378	391	13	-4.46	-4.66	-0.20	-5.54	-1.08
13	5-Ethyl-5-octylbarbiturate	386	391	5	-3.94	-4.21	-0.27	-5.00	-1.06
14	5-Ethyl-5-pentylbarbiturate	408	392	16	-2.34	-2.93	-0.59	-3.15	-0.81
15	5-Ethyl-5-propylbarbiturate	417	409	8	-1.49	-2.00	-0.51	-1.98	-0.49
16	5-Ethyl-barbiturate	464	479	15	-0.92	-1.07	-0.15	-1.66	-0.73
17	5-i-Propyl-5-(3-methylbut-2-enyl) barbiturate	404	472	68	-2.59	-2.77	-0.18	-2.63	-0.04
18	5-Methyl-5-(3-methylbut-2-enyl) barbiturate	466	466	0	-2.60	-2.53	0.08	-1.59	1.01
19	5-Methyl-5-allylbarbiturate	440	438	2	-1.16	-1.34	-0.18	-0.43	0.73

20	5-Methyl-5-ethylbarbiturate	489	458	31	-1.23	-1.70	-0.48	-0.91	0.31
21	5-Methylbarbiturate	493	479	14	-1.13	-0.85	0.27	-0.86	0.27
22	5-t-Butyl-5-(3-methylbut-2-enyl) barbiturate	485	475	10	-3.55	-3.99	-0.44	-3.07	0.48
23	Allobarbital	445	400	45	-2.08	-1.89	0.19	-0.55	1.53
24	Amobarbital	430	417	13	-2.62	-3.00	-0.38	-3.02	-0.40
25	Aprobarbital	415	446	31	-1.71	-1.95	-0.23	-1.48	0.24
26	Barbituric acid	521	482	39	-0.96	-0.60	0.36	0.17	1.12
27	Butalbital	413	423	10	-2.12	-2.44	-0.32	-2.07	0.05
28	Butethal	398	392	6	-1.75	-2.32	-0.58	-2.46	-0.72
29	Cyclobarbital	446	461	15	-2.27	-2.48	-0.21	-2.93	-0.65
30	Cyclopentobarbital	413	460	47	-2.46[p]	-1.64	0.82	-1.71	0.74
31	Heptabarbital	448	480	32	-3.00	-3.03	-0.03	-3.66	-0.66
32	Heptobarbital	499	481	18	-2.38	-1.53	0.85	-1.59	0.79

33	Hexethal	398	391	7	-3.05	-3.34	-0.29	-3.80	-0.75
34	Idobutal	401	381	20	-2.17	-2.48	-0.30	-2.09	0.08
35	Isopropylbarbiturate	489	523	34	-1.46	-1.68	-0.22	-2.11	-0.65
36	Pentobarbital	402	417	16	-2.45	-2.71	-0.26	-3.02	-0.57
37	Phenobarbital	448	452	4	-2.31	-1.53	0.78	-2.18	0.13
38	Probarbital	471	465	6	-2.19	-2.39	-0.20	-1.95	0.23
39	Reposal	486	463	23	-2.77	-3.48	-0.71	-4.11	-1.34
40	Secbutabarbital	441	439	2	-2.26	-2.60	-0.33	-2.51	-0.24
41	Secobarbital	368	404	36	-2.33	-2.50	-0.17	-2.62	-0.29
42	Talbutal	382	423	41	-2.02	-2.13	-0.11	-2.07	-0.05
43	Vinbarbital	438	400	38	-2.46	-2.14	0.32	-2.23	0.23
44	Vinylbital	364	408	44	-2.32 [p]	-1.34	0.98	-2.49	-0.17

[p] Values obtained from ACD/Lab Software V11.02

In Tables 5.2 and 5.3, the first column shows the atomic composition of the groups considered and the first row gives the following the environmental descriptors.

X the group is bonded only to sp^3 hybrid atoms;

Y the group is singly bonded to sp^2 hybrid atom;

RG the group is within an aliphatic ring;

AR the group is within aromatic ring;

FU the group is a bridge-head in an aliphatic ring system;

H the group is bonded to H atom

Barb the value for whole barbituric acid ring

Table 5.2 Group Contribution Coefficients (J/mol) for the Calculation of Total Enthalpy of Melting

Group	**X**	**Y**	**RG**	**AR**	**FU**	**H**
-CH_3	1183	1785	-	-	-	-
-CH_2	1906	684	1319	-	-	-
*-CH_2**	4000	-	-	-	-	-
-CH	1047	-1545	836	1387	1127	-
-C	-85	-2246	-519	1219	1152	-
=CH_2	1371	-	-	-	-	-
=CH	1667	1399	973	-	-	-
=C	1296	-1005	531	-	-	-
-Barb	***20859***	***18578***	**-**	**-**	**-**	***23207***

Table 5.3 Group Contribution Coefficients for the Calculation of Total Logarithm Aqueous Activity

Group	***X***	***Y***	***RG***	***AR***	***FU***	***H***
$-CH_3$	0.958	0.711	-	-	-	-
$-CH_2$	0.687	0.334	0.520	-	-	-
$(-CH_2)^2$	-0.018	-	-	-	-	-
-CH	-0.100	-0.342	0.254	0.312	0.513	-
-C	-0.662	-0.890	-0.291	0.112	-	-
$=CH_2$	0.627	-	-	-	-	-
=CH	0.284	0.290	0.269	-	-	-
=C	-0.044	-0.230	0.087	-	-	-
-Barb	***-3.212***	***-2.901***	**-**	**-**	**-**	***-1.716***

Each compound was broken down into the groups using the same molecular fragmentation scheme described by Lian and Yalkowsky [246]. Microsoft Excel 2012 was used to perform all calculations for group counts, enthalpies of melting, entropies of melting, and aqueous activity coefficients. The barbiturate compounds are subdivided into three different groups based on whether they contain hydrogen, only sp3 atoms or at least one sp2 atoms at 5-position. These are designated as H-Barb, X-Barb, and Y-Barb, respectively (Figure 5.1). The mi and qi contributions of barbiturate rings were generated by subtracting the hydrocarbon group values in Tables 5.2 and 5.3 from the observed values.

5.4.2 Calculation of Melting Point by UPPER

For each compound, the total entropy of melting (ΔS_m) was estimated by Equation 5.17. The total enthalpy of melting (ΔH_m) for each barbiturate compound was calculated by multiplying the experimental melting point (T_m^{Obs}) by the calculated entropy of melting. The enthalpy of hydrocarbon groups ($\sum n_i m_i$) were obtained from Lian and Yalkowsky [246]. The mean enthalpy m_i^{barb} values for H-Barb, X-Barb, and Y-Barb (Table 5.2.) were obtained from the difference between the calculated total enthalpy and the sum of the hydrocarbon values. Finally, the total enthalpies for predicting melting point were obtained by adding the calculated m_i^{barb} value to the hydrocarbon group values. These calculated enthalpy and entropy values were used to calculate melting point T_m^{Calc} via Equation 5.23.

$$T_m^{Calc} = \frac{\Delta H_m}{\Delta S_m} = \frac{\sum n_i m_i + m_i^{barb}}{43.54 - 8.95 \log \sigma + 7.93\ \Phi + 9.16 \log \varepsilon_{ar} + 9.43 \log \varepsilon_{al}} \quad \text{(Equation 5.23)}$$

where m_i^{barb} is the group contribution value for one of the three above-mentioned barbituric acid rings to the total enthalpy of melting.

5.4.3 Calculation of Solubility by UPPER

The effect of solute crystallinity is determined by incorporating the calculated entropy of melting and the calculated melting point into Equation 5.18. The aqueous activity coefficient for each compound was calculated by adding the q_i^{barb} value for the ring to the sum of the hydrocarbon group values. These equations are combined to give

$$\log S_w^{Calc} = - \frac{(43.54 - 8.95 \log \sigma + 7.93\ \Phi + 9.16 \log \varepsilon_{ar} + 9.43 \log \varepsilon_{al})\ (T_m^{Calc} - T)}{2.303\ RT} - (\sum n_i q_i + q_i^{barb})$$

(Equation 5.24)

The total aqueous activity coefficient for each barbiturate compound was calculated using Equation 5.21. The aqueous activity coefficients of the hydrocarbon groups ($\sum q_i m_i$) were calculated by adding group q_i values from Lian and Yalkowsky [246]. The aqueous activity coefficients q_i^{barb} values for H-Barb, X-Barb, and Y-Barb (Table 5.3) were obtained from the difference between calculated total aqueous activity coefficient and the sum of the hydrocarbon values. As shown in Equation 5.24, the final calculated log γ_w for predicting

solubility was obtained by adding the q_i^{barb} values and other substituted group values and these values were used to calculate log S_w^{Calc}.

5.4.4 Calculation of Solubility by the GSE

The General Solubility Equation (GSE) of Yalkowsky provides a simple means of estimating the aqueous solubility of nonelectrolytes in which the logarithm of the octanol-water partition coefficient is used to represent the aqueous activity coefficient, and Equation 5.20 is used as the ideal solubility. Thus,

$\log S_w$ = 0.5 – log P - 0.01 (MP- 25) (Equation 5.25)

where P is the octanol-water partition coefficient.

5.5 Results and Discussion

5.5.1 Melting Point

The observed and predicted melting points of the barbiturates are shown in Figure 5.2. Note that the negative and positive residual values of Table 5.1 correspond to underestimates and overestimates in the prediction, respectively. In order to calculate the total enthalpy of classical barbiturates, we need to calculate enthalpic group contribution of the barbiturate ring as the UPPER model of hydrocarbons does not account for the non-hydrocarbon moiety. The melting points were generated by incorporating the group m_i values of Lian and Yalkowsky along with the appropriate barbituric acid ring coefficient. Note that these three m_i^{barb} values are the only regression- generated enthalpic parameters used to predict melting points. The average absolute error (AAE) in the prediction of melting points is 20.6° for 44 barbiturates

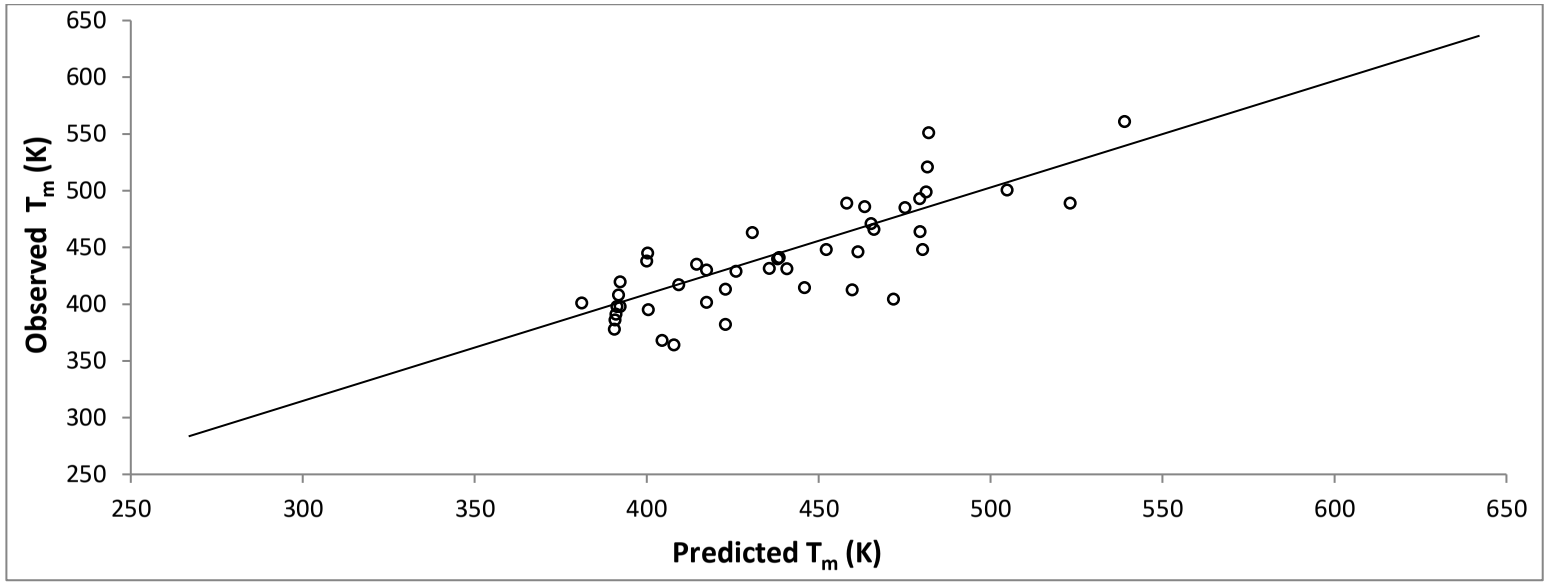

Figure 5.2 Observed vs. Predicted Melting Point (K). (**o**) All Barbiturates Compounds Used in the Training Dataset to Generate m_i^{barb} Values and (–) the Line of Identity.

5.5.2 Aqueous Solubility

The observed and predicted logarithms of the aqueous solubility by the UPPER model are shown in Figure 5.3. Again, the new entropic descriptors and only one of the three fitted q_i^{barb} values used to predict solubility of each compound. The average absolute error for predicting aqueous solubility using the UPPER and GSE models are 0.57 and 0.38, respectively. As shown in Figure 5.3, these predicted solubility values are in a good agreement with the experimental values. As expected, the GSE model can predict the solubility of barbiturates more accurately, as it uses observed melting point, which might not be available for all compounds in the early stages of drug discovery. UPPER, on the other hand, requires no experimental data and thus can be used in drug design.

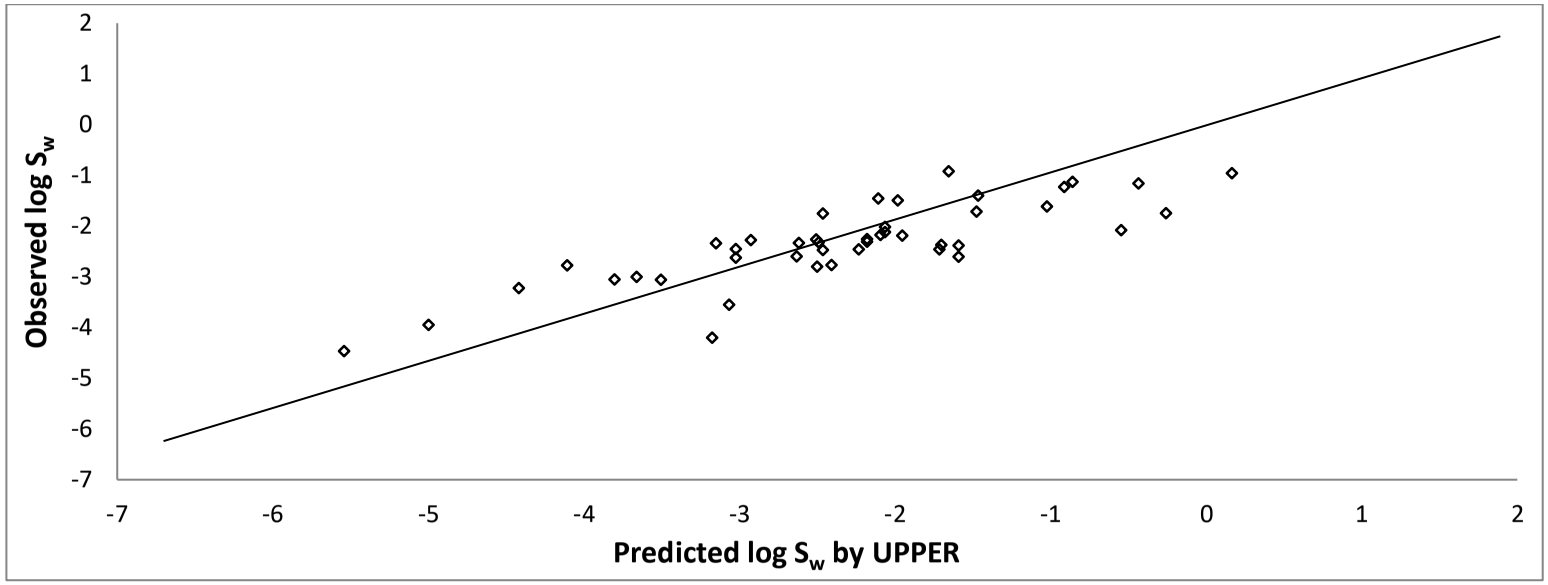

Figure 5.3 Observed vs. Predicted Logarithm Aqueous Solubility by UPPER. (◇) All Barbiturates Compounds Used in the Training Dataset to Generate q_i^{barb} Values and (–) the line of Identity.

Table 5.4 Statistical Results for Melting Point and Aqueous Solubility

Properties	Average Absolute Error
$\boldsymbol{T_m^{Calc}}$	20.6
log $\boldsymbol{S_w^{Calc}}$ by UPPER	0.57
log $\boldsymbol{S_w^{Calc}}$ by GSE	0.38

5.6 Conclusion

The UPPER model, which is developed on the basis of simple hydrocarbons is applied to barbiturates. The prediction of properties is directly based on the chemical structure and well-known thermodynamic relationships. It is clear from the results listed in Table 5.4 that there is a good agreement between the predicted and observed values. Thus, this simple and efficient approach could be useful for predicting melting points and aqueous solubility of novel barbiturates and other compounds for which the experimental values are unavailable.

APPENDIX A- SUPPLEMENTARY DATA

Table A.1 Physical Properties, Dose, Human Intestinal Absorption Data,

and calculated absorption parameter Π for Drugs used in Chapter 3

Name	CAS NO	FA	Ref for FA	log P	Ref For log P	MW	Ref for MW	log S	Ref for log S	Dose (D) in mole	Ref for dose	O Lumen	Π
Arbekacin	51025-85-5	0	38	-4.24	55	552.6	55	0.26	55	3.6E-04	41	1.0E+00	-4.24
Azlocillin	37091-66-0	0	38	0.83	55	461.5	55	-4.14	55	1.3E-02	41	7.1E+02	-2.02
Cefodizime	69739-16-8	0	38	0.52	55	584.7	55	-5.10	55	3.4E-03	41	1.7E+03	-2.71
Gentamicin C1	25876-10-2	0	38	-2.04	55	477.6	55	0.32	55	3.8E-04	41	1.0E+00	-2.04
Gentamicin C1a	26098-04-4	0	38	-2.93	55	449.5	55	0.35	55	4.0E-04	41	1.0E+00	-2.93
Meropenem	96036-03-2	0	38	-1.23	55	383.5	55	-1.89	55	1.6E-02	43	4.8E+00	-1.91
Mezlocillin	51481-65-3	0	38	0.33	55	539.6	55	-4.42	55	3.0E-02	41	3.1E+03	-3.17
Netilmicin	56391-56-1	0	38	-1.84	55	475.6	55	0.32	55	9.5E-04	42	1.0E+00	-1.84
Pentamidine	100-33-4	0	38	2.85	55	340.4	55	-4.05	55	7.1E-04	41	3.2E+01	1.35

Raffinose	000512-69-6	0	38	-5.10	55	504.4	55	-0.70	55	1.6E-02	3	1.0E+00	-5.10
Streptozocin	18883-66-4	0	38	-1.33	55	265.2	55	-0.77	55	2.4E-02	41	1.0E+00	-1.33
Tobramycin	32986-56-4	0	38	-4.22	55	467.5	55	0.33	55	1.2E-03	41	1.0E+00	-4.22
Vancomycin	1404-90-6	0	38	-1.41	55	1449.3	55	-7.10	55	1.4E-03	43	7.0E+04	-6.25
Alendronic acid	66376-36-1	0.01	38	-0.73	55	249.1	55	0.34	55	1.6E-04	41	1.0E+00	-0.73
Aztreonam	78110-38-0	0.01	38	0.49	55	435.4	55	-4.07	55	1.8E-02	41	8.6E+02	-2.45
Ceftriaxone	73384-59-5	0.01	38	-0.68	55	554.6	55	-4.72	55	7.2E-03	41	1.5E+03	-3.87
Lactulose	4618-18-2	0.01	38	-2.97	55	342.3	55	-0.51	55	1.2E-01	43	1.5E+00	-3.14
Risedronic acid	105462-24-6	0.01	38	0.55	55	283.1	55	-0.70	55	1.8E-05	41	1.0E+00	0.55
Streptomycin A	57-92-1	0.01	38	-1.22	55	581.6	55	-2.92	55	2.1E-03	41	6.9E+00	-2.06
Acarbose	56180-94-0	0.02	38	-7.91	55	645.6	55	-0.96	55	4.6E-04	43	1.0E+00	-7.91
Amphotericin B	1397-89-3	0.03	38	2.30	55	924.1	55	-2.15	55	9.7E-05	41	1.0E+00	2.30
Clodronate	10596-23-3	0.03	38	-2.38	57	244.9	55	0.09	57	1.3E-02	43	1.0E+00	-2.38
Nedocromil	69049-73-6	0.03	38	1.30	55	371.3	55	-5.55	55	3.8E-05	41	5.4E+01	-0.43
Neomycin	1404-04-2	0.03	38	-2.78	57	628.7	55	-1.32	57	9.5E-03	41	1.0E+00	-2.78
Amygdalin	29883-15-6	0.05	38	-2.24	55	457.4	55	-1.72	55	1.1E-03	41	1.0E+00	-2.24
Cefotaxime	63527-52-6	0.05	38	-0.51	55	453.5	55	-3.70	55	2.6E-02	41	5.3E+02	-3.23

Chlorhexidine	55-56-1	0.05	38	4.58	55	505.5	55	-5.70	55	7.1E-05	42	1.4E+02	2.42
Diatrizoate	117-96-4	0.05	38	0.49	55	613.9	55	-2.89	55	4.7E-02	41	1.5E+02	-1.67
Edetic acid	60-00-4	0.05	38	-0.84	55	292.2	55	0.53	55	1.4E-02	41	1.0E+00	-0.84
Etidronate	2809-21-4	0.05	38	-0.75	55	206.0	55	0.37	55	5.8E-03	41	1.0E+00	-0.75
Imipenem	64221-86-9	0.05	38	-2.95	55	299.4	55	-0.54	55	1.3E-02	41	1.0E+00	-2.95
Iohexol	66108-95-0	0.05	38	-2.92	55	821.1	55	-1.74	55	8.0E-03	41	1.8E+00	-3.17
Iotroxic acid	51022-74-3	0.05	38	4.32	55	1215.8	55	-5.80	55	8.2E-03	41	2.1E+04	0.01
Mitoxantrone	65271-80-9	0.05	38	1.55	55	444.5	55	-4.46	55	4.5E-05	43	5.1E+00	0.84
Moexipril	103775-10-6	0.05	38	4.77	55	498.6	55	-4.46	55	1.0E-04	41	1.1E+01	3.71
Pamidronic acid	40391-99-9	0.05	38	-0.89	55	235.1	55	0.60	55	3.8E-04	41	1.0E+00	-0.89
Phthalylsulfathiazole	85-73-4	0.05	38	0.80	55	403.4	55	-4.41	55	3.0E-02	41	3.1E+03	-2.68
Succinylsulfathiazole	116-43-8	0.05	38	0.19	55	355.4	55	-2.59	55	4.2E-02	52	6.5E+01	-1.62
Sulbactam	68373-14-8	0.05	38	0.39	55	233.2	55	-2.06	55	1.7E-02	41	7.9E+00	-0.51
Ticarcillin	34787-01-4	0.05	38	1.24	55	384.4	55	-2.92	55	4.7E-02	41	1.6E+02	-0.95
Cefmetazole	56796-20-4	0.1	38	-0.62	55	471.5	55	-4.40	55	1.3E-02	41	1.3E+03	-3.73
Acamprosate	77337-76-9	0.11	38	-2.68	55	181.2	55	0.39	55	1.1E-02	43	1.0E+00	-2.68
Cilazaprilat	90139-06-3	0.2	38	2.68	55	389.5	55	-3.80	55	2.6E-05	43	1.0E+00	2.68

Lincomycin	154-21-2	0.28	38	0.72	55	406.5	55	-1.49	55	4.9E-03	41	1.0E+00	0.72
Netivudine	84558-93-0	0.28	38	-0.49	55	282.3	55	-2.23	55	7.1E-04	41	1.0E+00	-0.49
Fosmidomycin	66508-53-0	0.3	38	-1.63	55	183.1	55	0.21	55	6.6E-03	41	1.0E+00	-1.63
AAFC (Flurocitabine)	37717-21-8	0.32	38	-1.91	55	243.2	55	-1.17	55	4.9E-03	3	1.0E+00	-1.91
Nadolol	42200-33-9	0.32	38	0.56	55	309.4	55	-1.74	55	2.1E-03	41	1.0E+00	0.56
Dihydroergotamine	511-12-6	0.35	38	5.69	55	583.7	55	-5.14	55	3.4E-06	43	1.9E+00	5.42
Sulpiride	15676-16-1	0.4	38	0.78	55	341.4	55	-2.00	55	9.4E-03	42	3.7E+00	0.20
Famotidine	76824-35-6	0.41	38	-1.66	55	337.5	55	-2.26	55	1.2E-04	41	1.0E+00	-1.66
Metaproterenol	586-06-1	0.43	38	0.29	55	211.3	55	-0.24	55	3.8E-04	43	1.0E+00	0.29
Cymarin	508-77-0	0.47	38	0.66	55	548.7	55	-3.08	55	5.5E-06	3	1.0E+00	0.66
Rimiterol	32953-89-2	0.48	38	0.74	55	223.3	55	-0.54	55	2.1E-05	42	1.0E+00	0.74
Atenolol	29122-68-7	0.5	38	0.34	55	266.3	55	-1.31	55	7.5E-04	41	1.0E+00	0.34
Cefpodoxime proxetil	87239-81-4	0.5	38	2.95	55	557.6	55	-5.70	55	1.1E-03	41	2.2E+03	-0.39
Guanoxan	2165-19-7	0.5	38	0.83	55	207.2	55	-2.01	55	4.8E-05	41	1.0E+00	0.83
Trandolapril	87679-37-6	0.5	38	4.90	55	430.5	55	-4.41	55	7.4E-05	41	7.6E+00	4.02
Metformin	657-24-9	0.54	38	-1.25	55	129.2	55	0.31	55	2.3E-02	41	1.0E+00	-1.25
Eflornithine	70052-12-9	0.55	38	0.09	55	182.2	55	-0.01	55	1.3E-01	41	1.0E+00	0.09

Valsartan	137862-53-4	0.55	38	4.02	55	435.5	55	-5.00	55	7.3E-04	41	2.9E+02	1.55
Dipyridamole	58-32-2	0.58	38	3.35	55	504.6	55	-2.41	55	7.9E-04	43	1.0E+00	3.35
Oxytetracycline	79-57-2	0.58	38	0.48	55	460.4	55	-4.33	55	4.3E-03	41	3.7E+02	-2.09
Cilazapril	88768-40-5	0.59	38	2.21	55	417.5	55	-3.72	55	2.4E-05	43	1.0E+00	2.21
Fenoterol	13392-18-2	0.6	38	1.33	55	303.4	55	-1.54	55	5.3E-06	41	1.0E+00	1.33
Ivermectin	70288-86-7	0.6	38	6.92	57	887.1	55	-6.05	57	1.0E-05	41	4.6E+01	5.26
Oxycodone	76-42-6	0.6	38	1.59	55	315.4	55	-2.24	55	1.0E-03	41	1.0E+00	1.59
Pirbuterol	38677-81-5	0.6	38	0.04	55	240.3	55	-0.10	55	1.0E-05	43	1.0E+00	0.04
Ramipril	87333-19-5	0.6	38	4.37	55	416.5	55	-4.22	55	4.8E-05	41	3.2E+00	3.87
Ziprasidone	146939-27-7	0.6	38	2.97	55	412.9	55	-4.82	55	3.9E-04	41	1.0E+02	0.96
Furosemide	54-31-9	0.61	38	2.30	55	330.7	55	-4.04	55	1.8E-03	41	8.0E+01	0.40
Sulphasalazine	599-79-1	0.13	39	3.05	55	398.4	55	-5.24	55	2.0E-02	41	1.4E+04	-1.09
Terbutaline	23031-25-6	0.63	38	0.70	55	225.3	55	-0.55	55	6.7E-05	41	1.0E+00	0.70
Chlorthalidone	77-36-1	0.65	38	0.70	55	338.8	55	-3.14	55	1.5E-04	41	1.0E+00	0.70
Tolrestat	82964-04-3	0.66	38	3.59	55	357.4	55	-4.96	55	5.6E-04	41	2.0E+02	1.28
Hydroflumethiazide	135-09-1	0.67	38	0.08	55	331.3	55	-2.33	55	6.0E-04	41	1.0E+00	0.08
Sumatriptan	103628-46-2	0.67	38	0.44	55	295.4	55	-2.52	55	4.1E-05	41	1.0E+00	0.44

Mibefradil	116644-53-2	0.69	38	6.21	55	479.6	55	-5.43	55	2.1E-04	41	2.3E+02	3.86
Anagrelide	68475-42-3	0.7	38	2.13	55	256.1	55	-3.82	55	3.9E-05	43	1.0E+00	2.11
Benserazide	322-35-0	0.7	38	-2.67	55	257.2	55	0.10	55	7.8E-04	41	1.0E+00	-2.67
Bromhexine	3572-43-8	0.7	38	4.80	55	376.1	55	-4.24	55	1.3E-04	41	8.8E+00	3.85
Etodolac	41340-25-4	0.7	38	3.42	55	287.4	55	-3.36	55	4.2E-03	42	3.8E+01	1.84
Famciclovir	104227-87-4	0.7	38	-0.12	55	321.3	55	-3.27	55	4.7E-03	41	3.5E+01	-1.65
Isocarboxazid	59-63-2	0.7	38	1.63	55	231.3	55	-2.62	55	2.6E-04	41	1.0E+00	1.63
Mianserin	24219-97-4	0.7	38	1.14	55	264.4	55	-2.77	55	3.4E-04	41	1.0E+00	1.14
Moxisylyte	54-32-0	0.7	38	3.17	55	279.4	55	-3.06	55	1.1E-03	41	5.3E+00	2.45
Pimozide	2062-78-4	0.7	38	5.76	55	461.6	55	-5.96	55	2.2E-05	41	7.9E+01	3.86
Recainam	74738-24-2	0.71	38	2.78	55	263.4	55	-3.43	55	5.7E-03	42	6.2E+01	0.99
Ceftizoxime	68401-81-0	0.72	38	-0.65	55	383.4	55	-3.42	55	1.6E-02	41	1.6E+02	-2.87
Cycloserine	68-41-7	0.72	38	-2.99	55	102.1	55	0.99	55	9.8E-03	41	1.0E+00	-2.99
Benzbromarone	3562-84-3	0.73	38	6.65	55	424.1	55	-6.37	55	7.1E-04	41	6.6E+03	2.83
Quetiapine	111974-69-7	0.73	38	2.60	55	383.5	55	-4.18	55	2.1E-03	41	1.3E+02	0.50
Almotriptan	154323-57-6	0.75	38	2.30	55	335.5	55	-3.89	55	7.5E-05	43	2.3E+00	1.94
Clavulanic acid	58001-44-8	0.75	38	-0.32	55	199.2	55	0.70	55	1.9E-03	41	1.0E+00	-0.32

Ketoconazole	65277-42-1	0.75	38	4.04	55	531.4	55	-4.32	55	7.5E-04	43	6.3E+01	2.25
Mesna	3375-50-6	0.75	38	-1.41	55	142.2	55	-0.19	55	1.7E-03	41	1.0E+00	-1.41
Oseltamivir	196618-13-0	0.75	38	1.71	55	312.4	55	-1.85	55	4.8E-04	43	1.0E+00	1.71
Primidone	125-33-7	0.75	38	0.83	55	218.3	55	-2.15	55	2.3E-03	41	1.3E+00	0.71
Ethylmorphine	76-58-4	0.77	38	1.90	55	301.4	55	-2.66	55	1.7E-04	41	1.0E+00	1.90
Pantoprazole	102625-70-7	0.77	38	1.57	55	383.4	55	-4.17	55	1.0E-04	41	6.2E+00	0.78
Sibutramine	106650-56-0	0.77	38	5.47	55	279.9	55	-4.43	55	5.4E-05	41	5.8E+00	4.70
Tolterodine	124937-51-5	0.77	38	5.23	55	325.5	55	-4.44	55	1.5E-03	41	1.6E+02	3.01
Guanabenz	5051-62-7	0.78	38	2.66	55	231.1	55	-3.34	55	2.8E-04	43	2.4E+00	2.28
Mefloquine	53230-10-7	0.78	38	2.00	55	378.3	55	-3.23	55	3.3E-03	43	2.2E+01	0.65
Urapidil	34661-75-1	0.78	38	1.64	55	387.5	55	-2.11	55	6.2E-04	42	1.0E+00	1.64
Zatebradine	85175-67-3	0.79	38	4.48	55	456.6	55	-4.33	55	1.6E-05	53	1.4E+00	4.33
Acetohexamide	968-81-0	0.8	38	2.44	55	324.4	55	-3.62	55	4.6E-03	41	7.7E+01	0.55
Allopurinol	315-30-0	0.8	38	-0.55	55	136.1	55	-2.77	55	5.9E-03	41	1.4E+01	-1.69
Carvedilol	72956-09-3	0.8	38	4.07	55	406.5	55	-5.28	55	6.2E-05	41	4.6E+01	2.41
Chlorpheniramine	132-22-9	0.8	38	2.97	55	274.8	55	-2.96	55	2.9E-05	41	1.0E+00	2.97
Clonazepam	1622-61-3	0.8	38	2.52	55	315.7	55	-4.12	55	2.5E-05	41	1.3E+00	2.40

Dantrolene	7261-97-4	0.8	38	1.07	55	314.3	55	-5.17	55	1.3E-03	41	7.5E+02	-1.81
Enoximone	77671-31-9	0.8	38	3.05	55	248.3	55	-3.80	55	1.5E-03	42	3.8E+01	1.47
Floxacillin	5250-39-5	0.8	38	2.89	55	453.9	55	-4.66	55	8.8E-03	41	1.6E+03	-0.31
Flunarizine	52468-60-7	0.8	38	5.59	55	404.5	55	-5.16	55	2.5E-05	43	1.4E+01	4.44
Fluoxetine	54910-89-3	0.8	38	3.93	55	309.3	55	-3.74	55	2.6E-04	41	5.7E+00	3.17
Guanadrel	40580-59-4	0.8	38	0.55	55	213.3	55	-1.80	55	1.9E-03	42	1.0E+00	0.55
Isoniazid	54-85-3	0.8	38	-0.77	55	137.1	55	0.00	55	4.4E-03	41	1.0E+00	-0.77
Itraconazole	84625-61-6	0.8	38	5.00	55	705.6	55	-6.85	55	8.5E-04	41	2.4E+04	0.61
Mesalamine	89-57-6	0.8	38	0.74	55	153.1	55	-1.12	55	2.6E-02	43	1.4E+00	0.60
Methadone	76-99-3	0.8	38	3.93	55	309.5	55	-3.82	55	9.7E-05	41	2.6E+00	3.52
Methoxyamphetamine	64-13-1	0.8	38	1.68	55	165.2	55	-1.54	55	3.0E-05	49	1.0E+00	1.68
Methylphenidate	113-45-1	0.8	38	2.31	55	233.3	55	-2.12	55	2.6E-04	41	1.0E+00	2.31
Modafinil	68693-11-8	0.8	38	1.18	55	273.4	55	-2.38	55	7.3E-04	41	1.0E+00	1.18
Nabumetone	42924-53-8	0.8	38	3.14	55	228.3	55	-3.57	55	8.8E-03	43	1.3E+02	1.03
Omeprazole	73590-58-6	0.8	38	2.36	55	345.4	55	-4.06	55	3.5E-04	41	1.6E+01	1.16
Oxamniquine	21738-42-1	0.8	38	2.02	55	279.3	55	-1.92	55	1.3E-02	41	4.3E+00	1.39
Pramipexole	104632-26-0	0.8	38	2.35	55	211.3	55	-2.28	55	2.8E-05	41	1.0E+00	2.35

Quinidine	56-54-2	0.8	38	2.82	55	324.4	55	-3.35	55	1.8E-03	41	1.6E+01	1.61
Riboflavin	83-88-5	0.8	38	0.10	55	376.4	55	-3.15	55	8.0E-05	41	1.0E+00	0.10
Terbinafine	91161-71-6	0.8	38	5.58	55	291.4	55	-5.74	55	5.6E-03	41	1.2E+04	1.49
Ticlopidine	55142-85-3	0.8	38	3.23	55	263.8	55	-3.52	55	9.5E-04	41	1.3E+01	2.13
Trimeprazine	84-96-8	0.8	38	5.04	55	298.5	55	-5.11	55	3.4E-04	41	1.7E+02	2.80
Trimipramine	739-71-9	0.8	38	4.71	55	294.4	55	-4.64	55	6.8E-04	41	1.2E+02	2.64
Retinol	68-26-8	0.8	38	6.08	55	286.5	55	-6.57	55	1.9E-04	41	2.8E+03	2.62
Flecainide	54143-55-4	0.81	38	3.19	55	414.3	55	-3.38	55	7.2E-04	41	6.9E+00	2.35
Aspirin	50-78-2	0.82	38	1.40	55	180.2	55	-1.96	55	2.2E-02	41	8.1E+00	0.49
Ibutilide	122647-31-8	0.82	38	3.72	55	384.6	55	-3.20	55	5.2E-06	42	1.0E+00	3.72
Methylprednisolone	83-43-2	0.82	38	2.17	55	374.5	55	-3.89	55	6.7E-04	41	2.1E+01	0.86
Mifobate	76541-72-5	0.82	38	0.31	55	358.7	55	-1.28	55	1.7E-03	3	1.0E+00	0.31
Albuterol	18559-94-9	0.83	38	0.69	55	239.3	55	-0.16	55	1.3E-04	41	1.0E+00	0.69
Milrinone	78415-72-2	0.83	38	1.27	55	211.2	55	-1.74	55	1.4E-05	41	1.0E+00	1.27
Nateglinide	105816-04-4	0.83	38	2.35	55	317.4	55	-3.35	55	1.1E-03	43	1.0E+01	1.34
Bromazepam	1812-30-2	0.84	38	2.28	55	316.2	55	-2.77	55	9.5E-05	43	1.0E+00	2.28
Acebutolol	37517-30-9	0.85	38	1.77	55	336.4	55	-2.40	55	3.6E-03	43	3.6E+00	1.22

Acetaminophen	103-90-2	0.85	38	0.48	55	151.2	55	-1.01	55	2.0E-02	41	1.0E+00	0.48
Chlorguanide	500-92-5	0.85	38	2.49	55	253.7	55	-3.05	55	7.9E-04	41	3.5E+00	1.94
Dolasetron	115956-12-2	0.85	38	2.57	55	324.4	55	-3.66	55	3.1E-04	43	5.6E+00	1.82
Isoproterenol	7683-59-2	0.85	38	0.32	55	211.3	55	-0.25	55	4.7E-05	41	1.0E+00	0.32
Lansoprazole	103577-45-3	0.85	38	2.58	55	369.4	55	-4.77	55	8.1E-05	41	1.9E+01	1.30
Quinine	130-95-0	0.85	38	2.82	55	324.4	55	-3.35	55	6.0E-03	43	5.3E+01	1.10
Oxyfedrine	15687-41-9	0.85	38	2.85	55	313.4	55	-3.00	55	1.5E-04	41	1.0E+00	2.85
Piretanide	55837-27-9	0.85	38	2.30	55	362.4	55	-3.70	55	3.3E-05	41	1.0E+00	2.30
Sulfamethizole	144-82-1	0.85	38	0.52	55	270.3	55	-2.70	55	1.5E-02	41	3.0E+01	-0.95
Triazolam	28911-01-5	0.85	38	2.08	55	343.2	55	-4.21	55	1.5E-06	43	1.0E+00	2.08
Zalcitabine	7481-89-2	0.85	38	-1.36	55	211.2	55	-1.00	55	1.1E-05	41	1.0E+00	-1.36
Lamivudine	134678-17-4	0.86	38	-0.51	55	229.3	55	-1.96	55	1.3E-03	41	1.0E+00	-0.51
Benzydamine	642-72-8	0.87	38	3.56	55	309.4	55	-4.18	55	1.2E-05	43	1.0E+00	3.56
Bupropion	34911-55-2	0.87	38	2.32	55	239.7	55	-2.74	55	1.9E-03	41	4.2E+00	1.70
Cimetidine	51481-61-9	0.87	38	-0.07	55	252.3	55	-2.54	55	9.5E-03	41	1.3E+01	-1.18
Clindamycin	18323-44-9	0.87	38	1.75	55	425.0	55	-2.00	55	4.2E-03	41	1.7E+00	1.52
Acrivastine	87848-99-5	0.88	38	2.41	55	348.4	55	-3.12	55	9.2E-05	41	1.0E+00	2.41

Disulfiram	97-77-8	0.88	38	3.82	55	296.5	55	-5.10	55	1.7E-03	41	8.5E+02	0.89
Metoclopramide	364-62-5	0.88	38	2.16	55	299.8	55	-2.52	55	2.0E-04	43	1.0E+00	2.16
Misoprostol	59122-46-2	0.88	38	3.80	55	382.5	55	-4.01	55	2.1E-06	41	1.0E+00	3.80
Moricizine	31883-05-3	0.88	38	2.36	55	427.5	55	-4.51	55	2.1E-03	41	2.7E+02	-0.07
Moxonidine	75438-57-2	0.88	38	0.33	55	241.7	55	-2.11	55	2.5E-06	42	1.0E+00	0.33
Nitrendipine	39562-70-4	0.88	38	3.81	55	360.4	55	-4.64	55	5.5E-05	41	9.6E+00	2.82
Trovafloxacin	147059-72-1	0.88	38	1.01	55	416.4	55	-3.52	55	7.2E-04	43	9.6E+00	0.02
Dihydrocodeine	125-28-0	0.89	38	0.61	55	301.4	55	-2.06	55	6.4E-04	41	1.0E+00	0.61
Sultopride	53583-79-2	0.89	38	1.39	55	354.5	55	-2.40	55	3.4E-03	41	3.4E+00	0.86
Tenidap	120210-48-2	0.89	38	1.59	55	320.8	55	-3.23	55	3.7E-04	42	2.5E+00	1.19
Almitrine	27469-53-0	0.9	38	6.11	55	477.6	55	-6.59	55	2.1E-04	43	3.2E+03	2.60
Amantadine	768-94-5	0.9	38	2.44	55	151.3	55	-2.42	55	2.6E-03	41	2.8E+00	2.00
Amphetamine	300-62-9	0.9	38	1.79	55	135.2	55	-1.42	55	4.4E-04	41	1.0E+00	1.79
Azatadine	3964-81-6	0.9	38	2.69	55	290.4	55	-2.77	55	6.9E-06	41	1.0E+00	2.69
Betaxolol	63659-18-7	0.9	38	2.53	55	307.4	55	-2.57	55	1.3E-04	41	1.0E+00	2.53
Bisoprolol	66722-44-9	0.9	38	1.89	55	325.4	55	-1.60	55	6.1E-05	41	1.0E+00	1.89
Chlorzoxazone	95-25-0	0.9	38	1.82	55	169.6	55	-2.15	55	1.2E-02	41	6.6E+00	0.99

Dapsone	80-08-0	0.9	38	0.99	55	248.3	55	-3.18	55	1.2E-03	41	7.3E+00	0.13
Dexamethasone	50-02-2	0.9	38	2.03	55	392.5	55	-4.05	55	2.3E-05	41	1.0E+00	2.02
Diethylstilbestrol	56-53-1	0.9	38	5.33	55	268.4	55	-4.60	55	2.2E-03	41	3.6E+02	2.78
Diflunisal	22494-42-4	0.9	38	3.65	55	250.2	55	-4.00	55	6.0E-03	41	2.4E+02	1.27
Diloxanide	579-38-4	0.9	38	1.67	55	234.1	55	-1.70	55	6.4E-03	41	1.3E+00	1.57
Ethacrynic acid	58-54-8	0.9	38	2.84	55	303.1	55	-3.64	55	1.3E-03	43	2.3E+01	1.48
Felbamate	25451-15-4	0.9	38	0.73	55	238.2	55	-1.80	55	1.5E-02	41	3.8E+00	0.15
Feprazone	30748-29-9	0.9	38	3.05	55	320.4	55	-3.85	55	2.3E-03	41	6.7E+01	1.22
Flutamide	13311-84-7	0.9	38	3.52	55	276.2	55	-3.89	55	2.7E-03	43	8.4E+01	1.60
Fluvoxamine	54739-18-3	0.9	38	3.71	55	318.3	55	-2.92	55	9.4E-04	43	3.1E+00	3.22
Hydroxyprogesterone caproate	630-56-8	0.9	38	5.68	55	428.6	55	-6.02	55	5.8E-04	43	2.5E+03	2.29
Isosorbide dinitrate	87-33-2	0.9	38	0.95	55	236.1	55	-2.20	55	1.0E-03	43	1.0E+00	0.95
Isotretinoin	4759-48-2	0.9	38	6.26	55	300.4	55	-4.68	55	4.0E-04	41	7.6E+01	4.38
Ketotifen	34580-13-7	0.9	38	2.19	55	309.4	55	-3.96	55	6.5E-06	41	1.0E+00	2.19
Loratadine	79794-75-5	0.9	38	3.90	55	382.9	55	-4.70	55	2.6E-05	41	5.2E+00	3.18
Mebeverine	3625-06-7	0.9	38	5.77	55	429.6	55	-4.96	55	9.4E-04	41	3.4E+02	3.23
Mefenamic acid	61-68-7	0.9	38	4.83	55	241.3	55	-4.29	55	5.2E-03	41	4.1E+02	2.23

Meloxicam	71125-38-7	0.9	38	2.66	55	351.4	55	-4.11	55	4.3E-05	43	2.2E+00	2.32
Mifepristone	84371-65-3	0.9	38	6.19	55	429.6	55	-7.89	55	1.4E-03	41	4.3E+05	0.56
Morphine	57-27-2	0.9	38	0.87	55	285.3	55	-1.82	55	3.5E-04	41	1.0E+00	0.87
Moxifloxacin	151096-09-2	0.9	38	2.83	55	401.4	55	-5.17	55	1.0E-03	43	5.9E+02	0.05
Nalidixic acid	389-08-2	0.9	38	0.03	55	232.2	55	-2.72	55	1.7E-02	41	3.6E+01	-1.53
Nisoldipine	63675-72-9	0.9	38	4.96	55	388.4	55	-5.34	55	1.0E-04	41	9.0E+01	3.00
Papaverine	58-74-2	0.9	38	2.93	55	339.4	55	-4.00	55	1.8E-03	41	7.1E+01	1.08
Phenazopyridine	94-78-0	0.9	38	2.21	55	213.2	55	-3.35	55	1.9E-03	41	1.7E+01	0.99
Phenytoin	57-41-0	0.9	38	1.42	55	252.3	55	-3.11	55	1.2E-03	41	6.2E+00	0.63
Prothionamide	14222-60-7	0.9	38	1.68	55	180.3	55	-1.92	55	2.8E-03	41	1.0E+00	1.68
Quinalbarbitone	76-73-3	0.9	38	2.30	55	238.3	55	-0.48	55	1.3E-03	43	1.0E+00	2.30
Rabeprazole	117976-89-3	0.9	38	2.10	55	359.4	55	-3.89	55	3.3E-04	43	1.0E+01	1.08
Riluzole	1744-22-5	0.9	38	2.92	55	234.2	55	-3.85	55	4.3E-04	43	1.2E+01	1.83
Sparfloxacin	110871-86-8	0.9	38	2.60	55	392.4	55	-5.12	55	1.0E-03	41	5.4E+02	-0.14
Sulfisomidine	515-64-0	0.9	38	0.58	55	278.3	55	-3.00	55	1.4E-02	41	5.7E+01	-1.18
Sulindac	38194-50-2	0.9	38	2.55	55	356.4	55	-4.48	55	1.1E-03	41	1.4E+02	0.42
Telithromycin	191114-48-4	0.9	38	5.22	55	812.0	55	-3.21	55	9.9E-04	43	6.5E+00	4.41

Thiabendazole	148-79-8	0.9	38	2.47	55	201.3	55	-3.52	55	1.5E-02	43	2.0E+02	0.17
Tiagabine	115103-54-3	0.9	38	4.03	55	375.6	55	-4.38	55	1.7E-04	41	1.6E+01	2.82
Tibolone	5630-53-5	0.9	38	3.52	55	312.5	55	-4.38	55	8.0E-06	41	1.0E+00	3.52
Tolazoline	59-98-3	0.9	38	1.80	55	160.2	55	-2.25	55	7.5E-04	41	1.0E+00	1.80
Triamcinolone acetonide	76-25-5	0.9	38	2.43	55	434.5	55	-4.00	55	2.3E-04	42	9.2E+00	1.46
Diltiazem	42399-41-7	0.91	38	4.73	55	414.5	55	-4.00	55	1.2E-03	41	4.6E+01	3.06
Hydrocortisone	50-23-7	0.91	38	1.76	55	362.5	55	-3.59	55	6.6E-04	43	1.0E+01	0.75
Naloxone	465-65-6	0.91	38	1.78	55	327.4	55	-2.29	55	1.8E-05	41	1.0E+00	1.78
Terazosin	63590-64-7	0.91	38	0.80	55	387.4	55	-3.64	55	5.2E-05	41	1.0E+00	0.80
Isradipine	75695-93-1	0.92	38	3.73	55	371.4	55	-4.70	55	2.7E-05	41	5.4E+00	3.00
Alprenolol	13655-52-2	0.93	38	2.91	55	249.4	55	-2.10	55	3.2E-03	42	1.6E+00	2.69
Amrinone	60719-84-8	0.93	38	-0.21	55	187.2	55	-0.85	55	2.4E-04	41	1.0E+00	-0.21
Scopolamine	51-34-3	0.93	38	0.69	55	303.4	55	-2.22	55	6.5E-08	41	1.0E+00	0.69
Tetrahydrocannabinol	1972-08-3	0.93	38	6.84	55	314.5	55	-5.60	55	6.4E-05	43	1.0E+02	4.83
Atropine	51-55-8	0.94	38	1.38	55	289.4	55	-2.06	55	2.8E-07	41	1.0E+00	1.38
Clozapine	5786-21-0	0.94	38	3.94	55	326.8	55	-4.85	55	2.8E-03	41	7.9E+02	1.04
Felodipine	72509-76-3	0.94	38	4.76	55	384.3	55	-5.28	55	5.2E-05	41	4.0E+01	3.16

Fluconazole	86386-73-4	0.94	38	0.45	55	306.3	55	-3.01	55	2.6E-03	43	1.1E+01	-0.58
Niacin	59-67-6	0.94	38	0.22	55	123.1	55	-0.29	55	6.1E-03	41	1.0E+00	0.22
Acipimox	51037-30-0	0.95	38	-1.00	55	154.1	55	0.33	55	4.9E-03	43	1.0E+00	-1.00
Amitriptyline	50-48-6	0.95	38	4.41	55	277.4	55	-3.92	55	1.1E-03	41	3.6E+01	2.85
Amobarbital	57-43-2	0.95	38	2.18	55	226.3	55	-2.68	55	4.4E-03	43	8.4E+00	1.25
Amoxapine	14028-44-5	0.95	38	2.93	55	313.8	55	-4.23	55	1.9E-03	41	1.3E+02	0.82
Baclofen	1134-47-0	0.95	38	0.78	55	213.7	55	-1.64	55	3.7E-04	41	1.0E+00	0.78
Carbimazole	22232-54-8	0.95	38	0.16	55	186.2	55	-1.20	55	3.2E-04	41	1.0E+00	0.16
Carteolol	51781-06-7	0.95	38	1.34	55	292.4	55	-1.41	55	3.4E-05	41	1.0E+00	1.34
Cephradine	38821-53-3	0.95	38	0.48	55	349.4	55	-3.24	55	1.1E-02	41	7.9E+01	-1.41
Chlorpropamide	94-20-2	0.95	38	2.30	55	276.7	55	-3.06	55	2.7E-03	41	1.2E+01	1.20
Clomethiazole	533-45-9	0.95	38	1.71	55	161.7	55	-2.17	55	2.4E-03	41	1.4E+00	1.55
Clomipramine	303-49-1	0.95	38	4.94	55	314.9	55	-5.05	55	7.9E-04	41	3.6E+02	2.39
Clonidine	4205-90-7	0.95	38	2.36	55	230.1	55	-3.12	55	1.0E-05	41	1.0E+00	2.36
Zuclopenthixol	53772-83-1	0.95	38	3.91	55	401.0	55	-3.72	55	2.5E-04	43	5.3E+00	3.19
Diethylpropion	90-84-6	0.95	38	2.55	55	205.3	55	-2.32	55	3.7E-04	41	1.0E+00	2.55
Disopyramide	3737-09-5	0.95	38	2.33	55	339.5	55	-3.24	55	4.7E-03	43	3.3E+01	0.81

Domperidone	57808-66-9	0.95	38	4.05	55	425.9	55	-5.46	55	7.0E-05	43	8.0E+01	2.14
Dothiepin	113-53-1	0.95	38	4.27	55	295.4	55	-3.89	55	5.1E-04	41	1.6E+01	3.07
Fludrocortisone acetate	514-36-3	0.95	38	2.72	55	422.5	55	-4.66	55	2.4E-07	41	1.0E+00	2.72
Flumazenil	78755-81-4	0.95	38	2.15	55	303.3	55	-3.85	55	9.9E-06	41	1.0E+00	2.15
Flurbiprofen	5104-49-4	0.95	38	3.66	55	244.3	55	-3.89	55	1.2E-03	43	3.8E+01	2.08
Galantamine	357-70-0	0.95	38	-0.05	55	287.4	55	-1.11	55	8.4E-05	43	1.0E+00	-0.05
Glymidine	339-44-6	0.95	38	-0.07	55	309.3	55	-2.47	55	6.5E-03	41	7.6E+00	-0.95
Hexobarbital	56-29-1	0.95	38	1.46	55	236.3	55	-2.30	55	2.1E-03	41	1.7E+00	1.23
Ketoprofen	22071-15-4	0.95	38	2.91	55	254.3	55	-3.37	55	1.2E-03	43	1.1E+01	1.87
Ketorolac	74103-06-3	0.95	38	2.68	55	255.3	55	-3.48	55	5.9E-04	41	7.1E+00	1.83
Levamisole	14769-73-4	0.95	38	1.84	55	204.3	55	-2.92	55	2.4E-04	41	1.0E+00	1.84
Lorazepam	846-49-1	0.95	38	2.38	55	321.2	55	-3.44	55	3.1E-05	41	1.0E+00	2.38
Methimazole	60-56-0	0.95	38	-0.34	55	114.2	55	-0.36	55	5.3E-04	41	1.0E+00	-0.34
Metronidazole	443-48-1	0.95	38	-0.14	55	171.2	55	-0.77	55	1.2E-02	41	1.0E+00	-0.14
Nicardipine	55985-32-5	0.95	38	4.89	55	479.5	55	-5.74	55	2.5E-04	41	5.6E+02	2.15
Nitrazepam	146-22-5	0.95	38	2.36	55	281.3	55	-3.54	55	7.1E-05	41	1.0E+00	2.36
Nitrofurantoin	67-20-9	0.95	38	-0.47	55	238.2	55	-3.52	55	1.7E-03	41	2.2E+01	-1.82

Nizatidine	76963-41-2	0.95	38	-0.49	55	331.5	55	0.48	55	9.1E-04	41	1.0E+00	-0.49
Pefloxacin	70458-92-3	0.95	38	1.92	55	333.4	55	-3.39	55	2.4E-03	43	2.3E+01	0.55
Pentazocine	359-83-1	0.95	38	4.15	55	285.4	55	-3.22	55	5.3E-04	41	3.5E+00	3.60
Pentoxifylline	6493-05-6	0.95	38	-0.15	55	278.3	55	-1.48	55	4.3E-03	41	1.0E+00	-0.15
Perindopril	82834-16-0	0.95	38	4.10	55	368.5	55	-3.34	55	2.2E-05	41	1.0E+00	4.10
Phenylpropanolamine	14838-15-4	0.95	38	0.36	55	151.2	55	-0.46	55	1.2E-03	41	1.0E+00	0.36
Practolol	6673-35-4	0.95	38	0.59	55	266.3	55	-1.21	55	2.3E-03	3	1.0E+00	0.59
Promethazine	60-87-7	0.95	38	4.89	55	284.4	55	-4.89	55	3.5E-04	41	1.1E+02	2.85
Propafenone	54063-53-5	0.95	38	3.35	55	341.4	55	-3.46	55	2.6E-03	43	3.0E+01	1.87
Propranolol	525-66-6	0.95	38	2.90	55	259.3	55	-2.74	55	2.5E-03	41	5.5E+00	2.16
Protriptyline	438-60-8	0.95	38	4.36	55	263.4	55	-3.70	55	2.3E-04	41	4.6E+00	3.70
Ritodrine	26652-09-5	0.95	38	2.04	55	287.4	55	-1.96	55	4.2E-04	42	1.0E+00	2.04
Sotalol	3930-20-9	0.95	38	0.24	55	272.4	55	-0.72	55	1.2E-03	41	1.0E+00	0.24
Sulfisoxazole	127-69-5	0.95	38	1.01	55	267.3	55	-3.12	55	1.5E-02	41	8.0E+01	-0.89
Tacrine	321-64-2	0.95	38	2.56	55	198.3	55	-3.26	55	8.1E-04	42	5.9E+00	1.79
Temazepam	846-50-4	0.95	38	2.19	55	300.7	55	-3.03	55	5.0E-05	41	1.0E+00	2.19
Timolol	26839-75-8	0.95	38	1.28	55	316.4	55	-2.85	55	1.9E-04	41	1.0E+00	1.28

Tropisetron	89565-68-4	0.95	38	3.03	55	284.4	55	-3.19	55	1.8E-05	43	1.0E+00	3.03
Venlafaxine	93413-69-5	0.95	38	2.48	55	277.4	55	-2.12	55	1.4E-03	41	1.0E+00	2.48
Zolpidem	82626-48-0	0.95	38	3.09	55	307.4	55	-3.38	55	3.3E-05	43	1.0E+00	3.09
Bumetanide	28395-03-1	0.96	38	2.88	55	364.4	55	-4.82	55	2.7E-05	41	7.3E+00	2.02
Clofibrate	637-07-0	0.96	38	3.88	55	242.7	55	-3.49	55	8.2E-03	41	1.0E+02	1.87
Gatifloxacin	112811-59-3	0.96	38	2.10	55	375.4	55	-4.29	55	1.3E-05	42	1.0E+00	2.09
Metoprolol	37350-58-6	0.96	38	1.63	55	267.4	55	-1.38	55	1.5E-03	41	1.0E+00	1.63
Minoxidil	51384-51-1	0.96	38	1.62	55	209.3	55	-3.24	55	4.8E-04	43	3.4E+00	1.09
Progesterone	57-83-0	0.96	38	3.83	55	314.5	55	-4.52	55	1.3E-03	43	1.7E+02	1.60
Torsemide	56211-40-6	0.96	38	1.96	55	348.4	55	-3.34	55	5.7E-04	41	5.0E+00	1.27
Trapidil	15421-84-8	0.96	38	2.31	55	205.3	55	-2.89	55	2.9E-03	43	9.0E+00	1.35
Cotinine	486-56-6	0.97	38	0.08	55	176.2	55	-0.89	55	1.1E-04	41	1.0E+00	0.08
Gallopamil	16662-47-8	0.97	38	3.83	55	484.6	55	-4.77	55	4.6E-04	42	1.1E+02	1.79
Gliclazide	21187-98-4	0.97	38	1.61	55	323.4	55	-3.54	55	9.9E-04	41	1.4E+01	0.48
Oxazepam	604-75-1	0.97	38	2.22	55	286.7	55	-2.85	55	4.2E-04	41	1.2E+00	2.14
Risperidone	106266-06-2	0.97	38	2.68	55	410.5	55	-4.55	55	3.9E-05	43	5.6E+00	1.93
Antipyrine	60-80-0	0.98	38	0.44	55	188.2	55	-1.09	55	3.2E-03	3	1.0E+00	0.44

Chlorpromazine	50-53-3	0.98	38	5.18	55	318.9	55	-5.49	55	3.1E-03	41	3.9E+03	1.59
Cisapride	81098-60-4	0.98	38	2.83	55	466.0	55	-4.11	55	1.7E-04	41	8.8E+00	1.89
Cyproterone acetate	427-51-0	0.98	38	4.22	55	416.9	55	-6.12	55	7.2E-04	41	3.8E+03	0.63
Glibornuride	26944-48-9	0.98	38	2.69	55	366.5	55	-3.66	55	1.4E-04	41	2.5E+00	2.29
Glyburide	10238-21-8	0.98	38	3.08	55	494.0	55	-5.10	55	4.0E-05	43	2.0E+01	1.76
Ibuprofen	15687-27-1	0.98	38	3.50	55	206.3	55	-3.04	55	1.2E-02	41	5.1E+01	1.80
Imatinib	152459-95-5	0.98	38	2.89	55	493.6	55	-4.77	55	1.6E-03	43	3.8E+02	0.31
Isoxepac	55453-87-7	0.98	38	2.11	55	268.3	55	-4.28	55	7.5E-04	41	5.7E+01	0.36
Lacidipine	103890-78-4	0.98	38	5.99	55	455.5	55	-5.96	55	1.8E-05	42	6.4E+01	4.18
Lamotrigine	84057-84-1	0.98	38	1.24	55	256.1	55	-3.24	55	1.6E-03	41	1.1E+01	0.20
Lidocaine	137-58-6	0.98	38	2.20	55	234.3	55	-2.21	55	1.3E-03	43	1.0E+00	2.20
Mexiletine	31828-71-4	0.98	38	2.12	55	179.3	55	-1.89	55	6.7E-03	43	2.1E+00	1.81
Nefopam	13669-70-0	0.98	38	1.91	55	253.3	55	-2.06	55	1.2E-03	42	1.0E+00	1.91
Oxaprozin	21256-18-8	0.98	38	3.15	55	293.3	55	-3.66	55	6.1E-03	43	1.1E+02	1.10
Pelrinone	94386-65-9	0.98	38	1.30	55	241.3	55	-3.18	55	4.1E-04	41	2.5E+00	0.90
Rivastigmine	123441-03-2	0.98	38	2.06	55	250.3	55	-1.00	55	4.8E-05	41	1.0E+00	2.06
Ropinirole	91374-21-9	0.98	38	2.49	55	260.4	55	-2.42	55	9.2E-05	42	1.0E+00	2.49

Tolmesoxide	38452-29-8	0.98	38	0.41	55	214.3	55	-1.48	55	1.9E-03	41	1.0E+00	0.41
Valproic acid	99-66-1	0.98	38	2.58	55	144.2	55	-1.80	55	1.7E-02	41	4.3E+00	1.94
Zopiclone	43200-80-2	0.98	38	2.71	55	388.8	55	-4.54	55	1.9E-05	43	2.7E+00	2.29
Caffeine	58-08-2	0.99	38	-0.63	55	194.2	55	-0.52	55	3.1E-03	41	1.0E+00	-0.63
Chlordiazepoxide	58-25-3	0.99	38	2.49	55	299.8	55	-0.68	55	3.3E-04	41	1.0E+00	2.49
Ciprofibrate	52214-84-3	0.99	38	2.93	55	289.2	55	-3.47	55	3.5E-04	41	4.1E+00	2.32
Diazepam	439-14-5	0.99	38	2.80	55	284.7	55	-3.74	55	1.4E-04	41	3.1E+00	2.31
Fluorescein	2321-07-5	0.99	38	2.68	55	332.3	55	-4.89	55	1.5E-03	43	4.6E+02	0.02
Lomefloxacin	98079-51-7	0.99	38	2.46	55	351.4	55	-4.17	55	1.1E-03	43	6.8E+01	0.63
Miconazole	22916-47-8	0.99	38	4.97	55	416.1	55	-5.68	55	8.7E-03	41	1.6E+04	0.76
Pheniramine	86-21-5	0.99	38	2.20	55	240.3	55	-2.18	55	1.6E-04	41	1.0E+00	2.20
Prednisolone	50-24-8	0.99	38	1.64	55	360.4	55	-3.55	55	5.5E-04	41	7.9E+00	0.74
Tiacrilast	78299-53-3	0.99	38	1.44	55	262.3	55	-2.85	55	2.9E-03	41	8.2E+00	0.52
Tianeptine	72797-41-2	0.99	38	4.13	55	437.0	55	-5.19	55	8.6E-05	43	5.3E+01	2.41
Viloxazine	46817-91-8	0.99	38	1.24	55	237.3	55	-1.49	55	1.9E-03	42	1.0E+00	1.24
Acetanilide	103-84-4	1	38	1.24	55	135.2	55	-1.44	55	2.2E-03	41	1.0E+00	1.24
Acetazolamide	59-66-5	1	38	-0.26	55	222.3	55	-1.89	55	4.5E-03	41	1.4E+00	-0.40

Alfacalcidol	41294-56-8	1	38	7.64	55	400.6	55	-6.25	55	4.5E-07	41	3.2E+00	7.13
Aminopyrine	58-15-1	1	38	0.85	55	231.3	55	-0.85	55	1.1E-03	3	1.0E+00	0.85
Amosulalol	85320-68-9	1	38	1.50	55	380.5	55	-2.70	55	3.9E-04	41	1.0E+00	1.50
Anastrozole	120511-73-1	1	38	0.29	55	293.4	55	-3.26	55	3.4E-06	41	1.0E+00	0.29
Astemizole	68844-77-9	1	38	5.52	55	458.6	55	-6.16	55	2.2E-05	41	1.3E+02	3.42
Azimilide	149908-53-2	1	38	3.33	55	458.0	55	-5.01	55	3.3E-04	41	1.4E+02	1.19
Bendroflumethiazide	73-48-3	1	38	1.29	55	421.4	55	-3.96	55	4.7E-05	41	1.7E+00	1.06
Benorylate	5003-48-5	1	38	2.15	55	313.3	55	-4.57	55	2.5E-02	41	3.8E+03	-1.43
Bepridil	64706-54-3	1	38	5.44	55	366.5	55	-4.92	55	1.1E-03	41	3.6E+02	2.88
Bezafibrate	41859-67-0	1	38	2.50	55	361.8	55	-3.82	55	1.7E-03	42	4.4E+01	0.86
Biperiden	514-65-8	1	38	4.27	55	311.5	55	-3.96	55	3.9E-05	41	1.4E+00	4.12
Bornaprine	20448-86-6	1	38	4.84	55	329.5	55	-4.46	55	3.6E-05	42	4.2E+00	4.22
Budesonide	51333-22-3	1	38	3.20	55	430.5	55	-4.66	55	6.0E-07	41	1.0E+00	3.20
Camazepam	36104-80-0	1	38	3.11	55	371.8	55	-3.68	55	5.4E-05	3	1.0E+00	3.10
Carbamazepine	298-46-4	1	38	1.90	55	236.3	55	-3.03	55	6.8E-03	41	2.9E+01	0.43
Carmustine	154-93-8	1	38	1.38	55	214.1	55	-1.70	55	2.3E-05	41	1.0E+00	1.38
Chloral hydrate	302-17-0	1	38	0.99	55	165.4	55	-0.59	55	1.2E-02	43	1.0E+00	0.99

Chloroquine	54-05-7	1	38	4.41	55	319.9	55	-4.57	55	3.1E-03	43	4.6E+02	1.75
Chlorphenesin	104-29-0	1	38	1.71	55	202.6	55	-1.85	55	1.2E-02	41	3.4E+00	1.18
Cicaprost	94079-80-8	1	38	3.06	55	374.5	55	-5.19	55	1.3E-07	41	1.0E+00	3.06
Cilomilast	153259-65-5	1	38	2.11	55	343.4	55	-3.74	55	8.7E-05	42	1.9E+00	1.82
Citalopram	59729-33-8	1	38	3.48	55	324.4	55	-4.52	55	1.8E-04	41	2.5E+01	2.08
Corticosterone	50-22-6	1	38	1.95	55	346.5	55	-3.55	55	6.9E-06	51	1.0E+00	1.95
Coumarin	91-64-5	1	38	1.39	55	146.1	55	-1.54	55	6.9E-04	41	1.0E+00	1.39
Cyclopenthiazide	742-20-1	1	38	2.23	55	379.9	55	-4.15	55	3.9E-06	41	1.0E+00	2.23
Diacetylmorphine	561-27-3	1	38	1.58	55	369.4	55	-3.49	55	9.7E-04	42	1.2E+01	0.49
Dicyclomine	77-19-0	1	38	4.64	55	309.5	55	-3.52	55	2.6E-04	41	3.4E+00	4.10
Dofetilide	115256-11-6	1	38	1.38	55	441.6	55	-2.68	55	2.3E-06	43	1.0E+00	1.38
Doxazosin	74191-85-8	1	38	2.85	55	451.5	55	-5.24	55	3.5E-05	41	2.4E+01	1.46
Ergotamine	113-15-5	1	38	7.37	55	581.7	55	-5.89	55	1.0E-05	43	3.2E+01	5.87
Ethinyl Estradiol	57-63-6	1	38	4.11	55	296.4	55	-4.89	55	1.0E-07	41	1.0E+00	4.11
Ethyl alcohol	64-17-5	1	38	-0.18	55	46.1	55	0.60	55	1.3E-01	41	1.0E+00	-0.18
Ethynodiol diacetate	297-76-7	1	38	5.45	55	384.5	55	-5.92	55	2.6E-06	41	8.7E+00	4.51
Fenclofenac	34645-84-6	1	38	4.59	55	297.1	55	-5.00	55	2.0E-03	41	8.1E+02	1.68

Finasteride	98319-26-7	1	38	3.83	55	372.5	55	-4.55	55	1.3E-05	41	1.9E+00	3.55
Flucytosine	2022-85-7	1	38	-1.40	55	129.1	55	0.26	55	7.0E-02	41	1.0E+00	-1.40
Flupenthixol	2709-56-0	1	38	3.67	55	434.5	55	-3.64	55	5.2E-04	42	9.0E+00	2.71
Fluvastatin	93957-54-1	1	38	4.57	55	411.5	55	-5.01	55	9.7E-05	41	4.0E+01	2.97
Fusidic acid	6990-06-3	1	38	5.76	55	516.7	55	-6.52	55	2.9E-03	41	3.9E+04	1.18
Gemfibrozil	25812-30-0	1	38	4.30	55	250.3	55	-3.60	55	4.8E-03	41	7.7E+01	2.42
Genaconazole	120924-80-3	1	38	1.48	55	331.3	55	-3.42	55	6.0E-04	41	6.4E+00	0.67
Glimepiride	93479-97-1	1	38	3.45	55	490.6	55	-5.26	55	1.6E-05	43	1.2E+01	2.37
Glipizide	29094-61-9	1	38	1.88	55	445.5	55	-3.13	55	9.0E-05	43	1.0E+00	1.88
Glycine	56-40-6	1	38	-0.93	55	75.1	55	1.12	55	8.0E-02	41	1.0E+00	-0.93
Granisetron	109889-09-0	1	38	2.91	55	312.4	55	-4.25	55	1.9E-06	41	1.0E+00	2.91
Haloperidol	52-86-8	1	38	3.76	55	375.9	55	-4.18	55	5.3E-05	43	3.2E+00	3.25
Hydralazine	86-54-4	1	38	0.95	55	160.2	55	-2.02	55	1.2E-03	41	1.0E+00	0.95
Indobufen	63610-08-2	1	38	3.33	55	295.3	55	-4.00	55	1.4E-03	43	5.4E+01	1.60
Indomethacin	53-86-1	1	38	4.25	55	357.8	55	-4.77	55	5.6E-04	43	1.3E+02	2.13
Irbesartan	138402-11-6	1	38	5.25	55	428.5	55	-6.19	55	7.0E-04	41	4.4E+03	1.60
Isosorbide-2-mononitrate	16051-77-7	1	38	-0.18	55	191.1	55	-0.74	55	6.3E-04	41	1.0E+00	-0.18

Isoxicam	34552-84-6	1	38	0.90	55	335.3	55	-2.85	55	6.0E-04	41	1.7E+00	0.67
Ketanserin	74050-98-9	1	38	3.56	55	395.4	55	-4.74	55	2.0E-04	41	4.5E+01	1.90
Letrozole	112809-51-5	1	38	0.43	55	285.3	55	-4.04	55	8.8E-06	41	1.0E+00	0.43
Levetiracetam	102767-28-2	1	38	-0.67	57	170.2	55	-0.83	57	2.1E-02	41	1.0E+00	-0.67
Levobunolol	47141-42-4	1	38	1.96	55	291.4	55	-2.72	55	4.6E-06	43	1.0E+00	1.96
Levonorgestrel	797-63-7	1	38	3.37	55	312.5	55	-4.27	55	4.8E-06	43	1.0E+00	3.37
Lisuride	18016-80-3	1	38	3.21	55	338.5	55	-3.49	55	1.5E-05	41	1.0E+00	3.21
Lormetazepam	848-75-9	1	38	2.35	55	335.2	55	-3.60	55	6.0E-06	42	1.0E+00	2.35
Lornoxicam	70374-39-9	1	38	0.77	55	371.8	55	-3.02	55	6.5E-05	43	1.0E+00	0.77
Lynestrenol	52-76-6	1	38	5.59	55	284.4	55	-5.64	55	1.8E-05	43	3.1E+01	4.10
Meclofenamic acid	644-62-2	1	38	5.44	55	296.2	55	-5.37	55	1.4E-03	43	1.3E+03	2.34
Megestrol acetate	595-33-5	1	38	3.75	55	384.5	55	-4.77	55	2.1E-03	43	4.9E+02	1.06
Meperidine	57-42-1	1	38	2.19	55	247.3	55	-1.82	55	3.6E-03	41	1.0E+00	2.19
Meptazinol	54340-58-8	1	38	3.40	55	233.4	55	-2.09	55	6.9E-03	42	3.4E+00	2.87
Methsuximide	77-41-8	1	38	0.42	55	203.2	55	-2.03	55	5.9E-03	41	2.5E+00	0.02
Methylergonovine	113-42-8	1	38	2.99	55	339.4	55	-3.04	55	2.4E-06	43	1.0E+00	2.99
Methysergide	361-37-5	1	38	1.81	55	353.5	55	-2.74	55	1.7E-05	41	1.0E+00	1.81

Midazolam	59467-70-8	1	38	3.80	55	325.8	55	-4.96	55	1.5E-05	41	5.6E+00	3.05
Nalbuphine	20594-83-6	1	38	1.00	55	357.4	55	-2.77	55	1.7E-04	41	1.0E+00	1.00
Nefazodone	83366-66-9	1	38	4.09	55	470.0	55	-5.29	55	1.3E-03	41	1.0E+03	1.09
Nicorandil	65141-46-0	1	38	0.74	55	211.2	55	-1.12	55	1.9E-04	43	1.0E+00	0.74
Nicotine	54-11-5	1	38	0.57	55	162.2	55	-0.42	55	4.9E-04	43	1.0E+00	0.57
Nilvadipine	75530-68-6	1	38	3.38	55	385.4	55	-5.14	55	4.2E-05	43	2.3E+01	2.02
Nitroxoline	4008-48-4	1	38	2.00	55	190.2	55	-2.55	55	3.2E-03	43	4.5E+00	1.35
Norethindrone	68-22-4	1	38	2.86	55	298.4	55	-4.00	55	3.4E-06	41	1.0E+00	2.86
Norgestimate	35189-28-7	1	38	5.13	55	369.5	55	-5.64	55	6.8E-07	43	1.2E+00	5.06
Nortriptyline	72-69-5	1	38	3.97	55	263.4	55	-3.60	55	3.8E-04	41	6.1E+00	3.19
Ofloxacin	82419-36-1	1	38	1.86	55	361.4	55	-3.72	55	2.2E-03	43	4.7E+01	0.19
Ondansetron	99614-02-5	1	38	1.56	55	293.4	55	-3.89	55	8.2E-05	41	2.5E+00	1.15
Orphenadrine	83-98-7	1	38	3.33	55	269.4	55	-2.96	55	1.5E-03	41	5.4E+00	2.59
Oxcarbazepine	28721-07-5	1	38	1.66	55	252.3	55	-3.11	55	4.8E-03	43	2.4E+01	0.27
Oxybutynin	5633-20-5	1	38	5.05	55	357.5	55	-4.59	55	5.6E-05	41	8.6E+00	4.11
Oxyphenbutazone	129-20-4	1	38	2.74	55	324.4	55	-3.66	55	3.1E-04	41	5.6E+00	1.99
Paroxetine	61869-08-7	1	38	3.70	55	329.4	55	-4.59	55	1.5E-04	41	2.3E+01	2.33

Pentobarbital	76-74-4	1	38	2.18	55	226.3	55	-2.70	55	8.8E-04	41	1.8E+00	1.93
Perphenazine	58-39-9	1	38	3.94	55	404.0	55	-4.17	55	5.9E-05	41	3.5E+00	3.40
Phenglutarimide	1156-05-4	1	38	1.89	55	288.4	55	-2.12	55	1.7E-04	41	1.0E+00	1.89
Phenindione	83-12-5	1	38	3.13	55	222.2	55	-4.60	55	9.0E-04	41	1.4E+02	0.97
Piroxicam	36322-90-4	1	38	0.59	55	331.4	55	-2.48	55	6.0E-05	43	1.0E+00	0.59
Polythiazide	346-18-9	1	38	2.05	55	439.9	55	-3.47	55	9.1E-06	43	1.0E+00	2.05
Probenecid	57-66-9	1	38	2.51	55	285.4	55	-3.06	55	3.5E-03	41	1.6E+01	1.31
Procarbazine	671-16-9	1	38	0.06	55	221.3	55	-1.42	55	1.6E-03	41	1.0E+00	0.06
Propofol	2078-54-8	1	38	3.66	55	178.3	55	-2.80	55	8.4E-04	41	2.1E+00	3.34
Proxyphylline	603-00-9	1	38	-0.56	55	238.2	55	-0.49	55	1.0E-02	41	1.0E+00	-0.56
Pseudoephedrine	90-82-4	1	38	1.08	55	165.2	55	-0.66	55	1.5E-03	41	1.0E+00	1.08
Pyrazinamide	98-96-4	1	38	-0.71	55	123.1	55	0.26	55	1.5E-02	41	1.0E+00	-0.71
Remoxipride	80125-14-0	1	38	2.19	55	371.3	55	-2.46	55	3.2E-03	42	3.7E+00	1.62
Repaglinide	135062-02-1	1	38	4.88	55	452.6	55	-4.72	55	3.5E-05	41	7.5E+00	4.00
Salsalate	552-94-3	1	38	2.76	55	258.2	55	-3.89	55	1.5E-02	41	4.8E+02	0.08
Selegiline	14611-51-9	1	38	2.68	55	187.3	55	-2.41	55	5.4E-05	41	1.0E+00	2.68
Sudoxicam	34042-85-8	1	38	2.36	55	337.4	55	-3.96	55	1.5E-04	44	5.4E+00	1.63

Sulfamethoxazole	723-46-6	1	38	0.66	55	253.3	55	-2.82	55	6.3E-03	43	1.7E+01	-0.57
Sulfinpyrazone	57-96-5	1	38	1.89	55	404.5	55	-4.28	55	2.0E-03	41	1.5E+02	-0.28
Tamoxifen	10540-29-1	1	38	5.13	55	371.5	55	-4.80	55	1.1E-04	43	2.7E+01	3.70
Tenoxicam	59804-37-4	1	38	0.01	55	337.4	55	-2.40	55	5.9E-05	43	1.0E+00	0.01
Terfenadine	50679-08-8	1	38	5.62	55	471.7	55	-5.49	55	2.5E-04	41	3.2E+02	3.11
Tesaglitazar	251565-85-2	1	38	1.55	55	408.5	55	-3.47	55	2.4E-06	41	1.0E+00	1.55
Testosterone	58-22-0	1	38	3.18	55	288.4	55	-4.15	55	3.5E-04	42	2.0E+01	1.88
Tilidine	51931-66-9	1	38	4.62	55	273.4	55	-3.18	55	7.3E-04	41	4.4E+00	3.98
Tinidazole	19387-91-8	1	38	-0.29	55	247.3	55	-1.89	55	8.1E-03	41	2.5E+00	-0.69
Tocainide	41708-72-9	1	38	0.81	55	192.3	55	-1.46	55	9.4E-03	43	1.1E+00	0.78
Toremifene	89778-26-7	1	38	4.77	55	406.0	55	-4.92	55	4.9E-04	41	1.6E+02	2.56
Triamcinolone	124-94-7	1	38	0.53	55	394.4	55	-3.22	55	2.5E-04	42	1.7E+00	0.30
Trifluoperazine	117-89-5	1	38	4.62	55	407.5	55	-4.74	55	9.8E-05	42	2.2E+01	3.28
Trihexyphenidyl	144-11-6	1	38	4.39	55	301.5	55	-3.35	55	5.0E-05	41	1.0E+00	4.39
Trofosfamide	22089-22-1	1	38	2.44	55	323.6	55	-2.14	55	9.3E-04	42	1.0E+00	2.44
Zileuton	111406-87-2	1	38	2.70	55	236.3	55	-3.62	55	1.0E-02	41	1.7E+02	0.48
Zomepirac	33369-31-2	1	38	3.36	55	291.7	55	-3.85	55	2.1E-03	41	5.9E+01	1.59

Zonisamide	68291-97-4	1	38	0.72	55	212.2	55	-2.44	55	2.8E-03	43	3.1E+00	0.22
Zotepine	26615-21-4	1	38	5.43	55	331.9	55	-4.85	55	1.4E-03	41	3.9E+02	2.85
Alcuronium	23214-96-2	0	38	-3.07	57	666.9	55	-0.90	57	2.7E-05	42	1.0E+00	-3.07
Atracurium	64228-79-1	0	38	1.04	57	929.1	55	-1.99	57	3.2E-05	41	1.0E+00	1.04
Cefpirome	84957-29-9	0	38	-2.05	57	475.5	55	-0.66	57	8.4E-03	43	1.0E+00	-2.05
Ceftazidime	72558-82-8	0	38	-2.84	57	547.6	55	-0.64	57	1.5E-02	41	1.0E+00	-2.84
Edrophonium	312-48-1	0	38	-2.58	57	166.2	55	0.22	57	2.5E-04	41	1.0E+00	-2.58
Mivacurium	106791-40-6	0	38	0.37	57	1029.3	55	-2.15	57	1.5E-05	42	1.0E+00	0.37
Pancuronium	16974-53-1	0	38	0.74	57	572.9	55	-1.12	57	1.0E-05	41	1.0E+00	0.74
Propantheline	298-50-0	0	38	-1.77	57	368.5	55	-0.35	57	1.2E-04	43	1.0E+00	-1.77
Tubocurarine	57-95-4	0	38	0.08	57	624.8	55	-1.13	57	6.4E-05	41	1.0E+00	0.08
Vecuronium	86029-43-8	0	38	1.79	57	557.8	55	-1.21	57	1.1E-05	41	1.0E+00	1.79
Neostigmine	59-99-4	0.02	38	-3.03	57	223.3	55	0.14	57	1.7E-03	41	1.0E+00	-3.03
Bephenium	7181-73-9	0.05	38	-0.49	57	256.4	55	-0.23	57	9.8E-03	41	1.0E+00	-0.49
Bethanechol	674-38-4	0.05	38	-3.95	57	161.2	55	0.39	57	1.2E-03	41	1.0E+00	-3.95
Gallamine triethiodide	65-29-2	0.05	38	-5.88	57	510.8	55	-0.20	57	2.3E-04	41	1.0E+00	-5.88
Ipratropium	60205-81-4	0.05	38	-2.21	57	332.5	55	-0.21	57	6.0E-06	43	1.0E+00	-2.21

Obidoxime	7683-36-5	0.05	38	-5.40	57	288.3	55	0.26	57	8.7E-04	42	1.0E+00	-5.40
Pentolinium	144-44-5	0.05	38	-2.74	57	240.4	55	0.07	57	4.2E-05	41	1.0E+00	-2.74
Diphemanil	62-97-5	0.07	38	2.20	57	278.4	55	-0.60	57	2.9E-03	41	1.0E+00	2.20
Butylscopolamine	7182-53-8	0.1	38	-1.99	57	360.5	55	-0.30	57	2.2E-04	41	1.0E+00	-1.99
Carnitine	541-15-1	0.1	38	-4.52	57	204.2	55	0.46	57	4.9E-03	41	1.0E+00	-4.52
Trospium	47608-32-2	0.1	38	0.70	57	408.6	55	-0.69	57	2.9E-05	41	1.0E+00	0.70
Oxitropium	99571-64-9	0.16	38	-2.36	57	332.4	55	-0.20	57	1.8E-06	43	1.0E+00	-2.36
Glycopyrrolate	13283-82-4	0.18	38	0.38	57	318.4	55	-0.48	57	1.3E-05	41	1.0E+00	0.38
Bretylium	59-41-6	0.23	38	-1.17	57	243.2	55	-0.12	57	1.2E-03	41	1.0E+00	-1.17
Pralidoxime	6735-59-7	0.3	38	-3.90	57	137.2	55	0.44	57	1.5E-02	41	1.0E+00	-3.90
Acitretin	55079-83-9	0.95	38	6.00	55	326.4	55	-4.89	55	2.3E-04	41	7.1E+01	4.15
Alprazolam	28981-97-7	0.9	38	1.92	55	308.8	55	-3.80	55	3.2E-05	41	1.0E+00	1.92
Amikacin	37517-28-5	0	38	-5.26	55	585.6	55	0.23	55	1.5E-03	41	1.0E+00	-5.26
Aminoglutethimide	125-84-8	1	38	0.54	55	232.3	55	-1.85	55	4.3E-03	41	1.2E+00	0.45
Azelastine	58581-89-8	1	38	3.47	55	381.9	55	-4.72	55	2.1E-05	41	4.4E+00	2.82
Betahistine	5638-76-6	1	38	-0.02	55	136.2	55	0.07	55	3.5E-04	41	1.0E+00	-0.02
Bicalutamide	90357-06-5	0.9	38	4.14	55	430.4	55	-5.74	55	1.2E-04	41	2.6E+02	1.72

Bifemelane	90293-01-9	0.95	38	3.97	55	269.4	55	-3.49	55	1.9E-04	41	2.3E+00	3.60
Buspirone	36505-84-7	1	38	1.59	55	385.5	55	-3.68	55	1.6E-04	41	3.0E+00	1.12
Capecitabine	154361-50-9	0.96	38	1.04	55	359.4	55	-3.17	55	1.1E-02	43	6.6E+01	-0.78
Chlorambucil	305-03-3	1	38	2.61	55	304.2	55	-3.72	55	3.9E-05	41	1.0E+00	2.61
Chloramphenicol	56-75-7	0.89	38	1.10	55	323.1	55	-2.48	55	1.9E-02	41	2.3E+01	-0.25
Cinchonine	118-10-5	1	38	2.79	55	294.4	55	-3.20	55	7.1E-03	54	4.5E+01	1.13
Cinoxacin	28657-80-9	0.95	38	0.49	55	262.2	55	-2.51	55	3.8E-03	41	4.9E+00	-0.20
Clobazam	22316-47-8	0.87	38	1.25	55	300.7	55	-3.64	55	2.7E-04	43	4.6E+00	0.59
Codeine	76-57-3	0.93	38	1.39	55	299.4	55	-2.31	55	1.2E-03	41	1.0E+00	1.39
Cyproheptadine	129-03-3	0.8	38	5.82	55	287.4	55	-4.43	55	1.0E-04	41	1.1E+01	4.77
Delmopinol	79874-76-3	0.95	38	3.89	55	271.4	55	-2.32	55	7.4E-06	41	1.0E+00	3.89
Desipramine	50-47-5	0.98	38	3.97	55	266.4	55	-4.07	55	1.1E-03	41	5.2E+01	2.25
Desmethyldiazepam	1088-11-5	0.99	38	2.78	55	270.7	55	-3.55	55	3.7E-05	41	1.0E+00	2.78
Desogestrel	54024-22-5	0.72	38	5.35	55	310.5	55	-5.41	55	4.8E-07	41	1.0E+00	5.35
Dextromoramide	357-56-2	1	38	2.53	55	392.5	55	-3.64	55	5.1E-05	41	1.0E+00	2.53
Diazoxide	364-98-7	0.9	38	1.19	55	230.7	55	-2.80	55	2.1E-03	41	5.2E+00	0.48
Diclofenac	15307-86-5	0.97	38	4.55	55	296.2	55	-4.89	55	7.6E-04	41	2.3E+02	2.18

Dienogest	65928-58-7	0.94	38	2.58	55	311.4	55	-3.89	55	6.4E-06	43	1.0E+00	2.58
Doxepin	1668-19-5	1	38	3.84	55	279.4	55	-3.77	55	1.1E-03	41	2.5E+01	2.43
Erythromycin	114-07-8	0.35	38	1.91	55	733.9	55	-1.30	55	5.5E-03	41	1.0E+00	1.91
Estramustine	2998-57-4	0.75	38	5.75	55	440.4	55	-6.74	55	2.2E-03	43	4.8E+04	1.06
Ethambutol	74-55-5	0.78	38	-0.29	55	204.3	55	0.46	55	7.3E-03	41	1.0E+00	-0.29
Ethionamide	536-33-4	0.9	38	1.17	55	166.2	55	-1.57	55	6.0E-03	41	1.0E+00	1.17
Etoricoxib	202409-33-4	1	38	2.46	55	358.8	55	-3.82	55	3.3E-04	43	8.9E+00	1.50
Fenfluramine	458-24-2	0.95	38	3.55	55	231.3	55	-2.77	55	5.2E-04	41	1.2E+00	3.47
Fenoprofen	29679-58-1	0.85	38	3.72	55	242.3	55	-3.85	55	1.2E-02	41	3.5E+02	1.17
Flunisolide	3385-03-3	0.8	38	2.04	55	434.5	55	-4.00	55	1.5E-06	43	1.0E+00	2.04
Flurazepam	17617-23-1	1	38	4.84	55	387.9	55	-5.04	55	7.7E-05	41	3.4E+01	3.32
Gestodene	60282-87-3	1	38	2.02	55	310.4	55	-3.41	55	2.4E-07	41	1.0E+00	2.02
Gliquidone	33342-05-1	0.95	38	3.91	55	527.6	55	-5.77	55	1.1E-04	41	2.7E+02	1.48
Guanfacine	29110-47-2	1	38	1.33	55	246.1	55	-2.72	55	1.2E-05	43	1.0E+00	1.33

Hydrochlorothiazide	58-93-5	0.68	38	-0.02	55	297.7	55	-2.22	55	6.7E-04	41	1.0E+00	-0.02
Hydroxychloroquine	118-42-3	0.9	38	3.53	55	335.9	55	-3.80	55	1.8E-03	41	4.5E+01	1.88
Imipramine	50-49-7	0.98	38	4.36	55	280.4	55	-4.35	55	1.1E-03	43	9.5E+01	2.38
Indoprofen	31842-01-0	1	38	2.82	55	281.3	55	-3.66	55	7.1E-04	41	1.3E+01	1.71
Kanamycin	59-01-8	0.01	38	-4.60	55	484.5	55	0.31	55	1.9E-03	41	1.0E+00	-4.60
Ketazolam	27223-35-4	1	38	0.51	55	368.8	55	-3.54	55	1.6E-04	43	2.2E+00	0.16
Labetalol	36894-69-6	0.95	38	2.72	55	328.4	55	-3.06	55	7.3E-03	41	3.3E+01	1.20
Levosimendan	141505-33-1	0.9	38	2.07	55	280.3	55	-4.66	55	5.0E-06	43	1.0E+00	2.07
Linezolid	165800-03-3	1	38	0.45	55	337.4	55	-2.96	55	3.6E-03	43	1.3E+01	-0.66
Losartan	114798-26-4	0.8	38	3.46	55	422.9	55	-5.25	55	2.4E-04	41	1.7E+02	1.23
Maprotiline	10262-69-8	0.98	38	4.36	55	277.4	55	-4.30	55	8.1E-04	43	6.5E+01	2.55
Mebendazole	31431-39-7	1	38	2.83	55	295.3	55	-4.85	55	6.8E-04	43	1.9E+02	0.54
Mestranol	72-33-3	0.9	38	4.94	55	310.4	55	-5.40	55	1.6E-07	41	1.0E+00	4.94
Methocarbamol	532-03-6	1	38	0.40	55	241.2	55	-1.19	55	2.5E-02	41	1.5E+00	0.22
Metolazone	17560-51-9	0.64	38	3.16	55	365.8	55	-4.92	55	5.5E-05	43	1.8E+01	1.90
Metyrapone	54-36-4	0.8	38	1.14	55	226.3	55	-1.89	55	2.0E-02	41	6.1E+00	0.35
Moclobemide	71320-77-9	0.88	38	1.34	55	268.7	55	-1.62	55	2.2E-03	43	1.0E+00	1.34

Moxalactam	64952-97-2	0	38	-2.56	55	520.5	55	-2.39	55	7.7E-03	41	7.5E+00	-3.44
Nafronyl	31329-57-4	1	38	3.91	55	383.5	55	-4.66	55	1.6E-03	41	2.8E+02	1.46
Naltrexone	16590-41-3	0.95	38	2.05	55	341.4	55	-3.00	55	4.4E-04	43	1.8E+00	1.80
Naproxen	22204-53-1	0.99	38	2.88	55	230.3	55	-3.33	55	6.5E-03	43	5.5E+01	1.13
Naratriptan	121679-13-8	0.7	38	1.15	55	335.5	55	-3.17	55	1.5E-05	41	1.0E+00	1.15
Nifedipine	21829-25-4	0.9	38	3.58	55	346.3	55	-4.47	55	5.2E-04	43	6.1E+01	1.80
Nilutamide	63612-50-0	1	38	1.94	55	317.2	55	-3.60	55	9.5E-04	43	1.5E+01	0.76
Norgestrel	6533-00-2	1	38	3.37	55	312.5	55	-4.27	55	1.6E-06	43	1.0E+00	3.37
Oxatomide	60607-34-3	1	38	4.34	55	426.6	55	-5.37	55	2.8E-04	43	2.6E+02	1.92
Oxprenolol	6452-71-7	0.95	38	2.15	55	265.4	55	-1.80	55	1.2E-03	42	1.0E+00	2.15
Penbutolol	38363-40-5	1	38	4.02	55	291.4	55	-3.15	55	2.7E-04	41	1.6E+00	3.83
Phenobarbital	50-06-6	1	38	0.53	55	232.2	55	-2.27	55	5.6E-04	41	1.0E+00	0.53
Phenprocoumon	435-97-2	0.95	38	4.64	55	280.3	55	-4.72	55	8.6E-05	41	1.8E+01	3.39
Phenylbutazone	50-33-9	0.98	38	3.38	55	308.4	55	-4.04	55	1.9E-03	41	8.6E+01	1.44
Pindolol	13523-86-9	0.9	38	1.68	55	248.3	55	-1.59	55	2.4E-04	41	1.0E+00	1.68
Piroximone	84490-12-0	0.81	38	1.86	55	217.2	55	-2.35	55	2.3E-04	41	1.0E+00	1.86
Pizotyline	15574-96-6	0.8	38	2.71	55	295.4	55	-3.59	55	1.0E-05	41	1.0E+00	2.71

Praziquantel	55268-74-1	0.96	38	2.66	55	312.4	55	-3.37	55	1.4E-02	43	1.3E+02	0.53
Procyclidine	77-37-2	1	38	3.86	55	287.4	55	-3.14	55	7.0E-05	41	1.0E+00	3.86
Propiverine	60569-19-9	0.84	38	4.37	55	367.5	55	-3.82	55	1.2E-04	43	3.3E+00	3.86
Propoxyphene	469-62-5	0.95	38	4.10	55	339.5	55	-4.07	55	1.1E-03	41	5.4E+01	2.36
Propylthiouracil	51-52-5	0.76	38	1.15	55	170.2	55	-2.62	55	5.3E-03	43	8.8E+00	0.21
Quinagolide	87056-78-8	1	38	4.12	55	395.6	55	-4.60	55	2.3E-06	43	1.0E+00	4.12
Reproterol	54063-54-6	0.6	38	-1.30	55	389.4	55	-0.68	55	1.5E-04	41	1.0E+00	-1.30
Rizatriptan	144034-80-0	0.9	38	1.20	55	269.3	55	-2.24	55	1.1E-04	41	1.0E+00	1.20
Saccharin	81-07-2	0.91	38	0.91	55	183.2	55	-2.08	55	1.1E-02	3	5.3E+00	0.19
Sorivudine	77181-69-2	0.82	38	-0.03	55	349.1	55	-2.52	55	4.3E-04	41	1.0E+00	-0.03
Stavudine	3056-17-5	1	38	-0.65	55	224.2	55	-1.70	55	3.6E-04	43	1.0E+00	-0.65
Sulfamethazine	57-68-1	0.95	38	0.30	55	278.3	55	-2.96	55	1.1E-02	41	3.9E+01	-1.30
Tamsulosin	106133-20-4	1	38	2.14	55	408.5	55	-3.62	55	2.0E-06	41	1.0E+00	2.14
Telmisartan	144701-48-4	0.9	38	6.48	55	514.6	55	-6.89	55	1.6E-04	41	4.8E+03	2.80
Tetrabenazine	58-46-8	1	38	2.93	55	317.4	55	-3.23	55	1.6E-04	42	1.1E+00	2.90
Tiludronic acid	89987-06-4	0.06	38	2.00	55	318.6	55	-3.01	55	1.3E-03	42	5.1E+00	1.29
Tolbutamide	64-77-7	0.9	38	2.36	55	270.4	55	-2.92	55	7.4E-03	41	2.5E+01	0.97

Tolmetin	26171-23-3	0.99	38	2.68	55	257.3	55	-3.24	55	7.0E-03	43	4.9E+01	0.99
Topiramate	97240-79-4	0.86	38	2.16	55	339.4	55	-3.55	55	1.2E-03	41	1.7E+01	0.93
Tramadol	27203-92-5	0.95	38	2.32	55	263.4	55	-1.82	55	1.5E-03	41	1.0E+00	2.32
Tranexamic acid	1197-18-8	0.55	38	0.50	55	157.2	55	-0.57	55	2.5E-02	43	1.0E+00	0.50
Trazodone	19794-93-5	1	38	2.76	55	371.9	55	-4.40	55	1.6E-03	43	1.6E+02	0.55
Trimethoprim	738-70-5	0.97	38	0.59	55	290.3	55	-2.77	55	1.1E-03	41	2.6E+00	0.18
Ximoprofen	56187-89-4	0.98	38	2.10	55	261.3	55	-2.72	55	1.1E-04	3	1.0E+00	2.10
Zaleplon	151319-34-5	1	38	1.40	55	305.3	55	-3.89	55	9.8E-05	41	3.0E+00	0.92
Zanamivir	139110-80-8	0.02	38	-1.87	55	332.3	55	-1.35	55	6.0E-05	41	1.0E+00	-1.87
Amoxicillin	26787-78-0	0.92	39	0.88	55	365.4	55	-1.96	55	4.1E-03	41	1.5E+00	0.71
Biotin	58-85-5	1	39	0.86	55	244.3	55	-3.52	55	8.2E-07	41	1.0E+00	0.86
Captopril	62571-86-2	0.84	39	1.99	55	217.3	55	-2.04	55	2.1E-03	43	1.0E+00	1.99
Cefatrizine	51627-14-6	0.75	39	-1.07	55	462.5	55	-3.46	55	2.2E-03	41	2.5E+01	-2.47
Cefuroxime	55268-75-2	0.445	39	0.26	55	424.4	55	-3.68	55	2.4E-03	41	4.5E+01	-1.39
Cefuroxime Axetil	64544-07-6	0.44	39	1.93	55	510.5	55	-4.96	55	2.0E-03	41	7.1E+02	-0.93
Folinic Acid	58-05-9	0.9	39	-1.43	55	473.4	55	-2.85	55	6.9E-04	41	2.0E+00	-1.72
Foscarnet	4428-95-9	0.18	39	-1.90	55	126.0	55	0.35	55	5.7E-02	41	1.0E+00	-1.90

Fosfomycin	23155-02-4	0.36	39	-1.23	55	138.1	55	-0.03	55	2.2E-02	43	1.0E+00	-1.23
Iothalamic acid	2276-90-6	0.02	39	-0.06	55	613.9	55	-2.33	55	9.8E-03	41	8.3E+00	-0.98
Methyldopa	555-30-6	0.5	39	-0.74	55	211.2	55	-0.23	55	9.5E-03	41	1.0E+00	-0.74
Molsidomine	25717-80-0	1	39	-0.87	57	242.2	55	-0.76	57	1.7E-04	42	1.0E+00	-0.87
Olsalazine	15722-48-2	0.08	39	3.57	55	302.2	55	-4.07	55	3.3E-03	41	1.5E+02	1.38
Prazosin	19216-56-9	0.86	39	2.14	55	383.4	55	-4.42	55	5.2E-05	43	5.5E+00	1.40
Quinapril	85441-61-8	0.6	39	4.79	55	438.5	55	-4.34	55	1.8E-04	41	1.6E+01	3.59
Abacavir	136470-78-5	0.83	39	1.16	55	286.3	55	-4.10	55	2.1E-03	43	1.1E+02	-0.87
Acyclovir	59277-89-3	0.23	39	-1.48	55	225.2	55	-1.85	55	3.5E-03	41	1.0E+00	-1.49
Adefovir	106941-25-7	0.16	39	-0.49	55	273.2	55	-1.70	55	3.7E-05	43	1.0E+00	-0.49
Albendazole	54965-21-8	0.05	39	3.00	55	265.3	55	-4.57	55	3.0E-03	41	4.5E+02	0.35
Amdinocillin	32887-01-7	0.05	39	2.33	55	325.4	55	-3.74	55	2.8E-03	41	6.1E+01	0.54
Amifostine	20537-88-6	1	39	-1.23	55	214.2	55	-0.24	55	6.9E-03	41	1.0E+00	-1.23
Amiloride	2609-46-3	0.5	39	0.93	55	229.6	55	-3.21	55	8.7E-05	43	1.0E+00	0.93
Ampicillin	69-53-4	0.62	39	1.48	55	349.4	55	-2.33	55	1.0E-02	41	8.5E+00	0.55
Antrafenine	55300-29-3	1	39	6.22	55	588.5	55	-6.20	55	5.1E-04	41	3.2E+03	2.71
Apricitabine	160707-69-7	0.8	39	-0.21	55	229.3	55	-2.11	55	3.5E-03	41	1.8E+00	-0.47

Aprindine	37640-71-4	0.85	39	5.68	55	322.5	55	-5.21	55	9.3E-04	41	6.0E+02	2.90
Aripiprazole	129722-12-9	0.87	39	3.76	55	448.4	55	-3.74	55	6.7E-05	43	1.5E+00	3.59
Ascorbic Acid	50-81-7	1	39	-2.78	55	176.1	55	0.75	55	3.4E-02	41	1.0E+00	-2.78
Bambuterol	81732-65-2	0.2	39	1.04	55	367.4	55	0.39	55	5.4E-05	43	1.0E+00	1.04
Benazepril	86541-75-5	0.5	39	4.54	55	424.5	55	-4.00	55	1.9E-04	41	7.5E+00	3.66
Betazole	105-20-4	1	39	-0.36	55	111.2	55	-0.68	55	2.7E-04	41	1.0E+00	-0.36
Bromocriptine	25614-03-3	0.28	39	8.60	55	654.6	55	-6.48	55	1.5E-04	41	1.9E+03	5.33
Brompheniramine	86-22-6	0.89	39	3.24	55	319.2	55	-3.00	55	7.5E-05	41	1.0E+00	3.24
Busulfan	55-98-1	1	39	-0.56	55	246.3	55	-1.52	55	3.2E-05	41	1.0E+00	-0.56
Carbamazepine10 11Epoxide	36507-30-9	0.9	39	0.16	55	252.3	55	-2.12	55	6.3E-03	43	3.3E+00	-0.37
Carfecillin	27025-49-6	0.99	39	2.85	55	454.5	55	-4.64	55	2.2E-03	41	3.8E+02	0.27
Carprofen	53716-49-7	1	39	3.84	55	273.7	55	-5.27	55	2.2E-03	43	1.6E+03	0.63
Cefaclor	53994-73-3	0.9	39	0.14	55	367.8	55	-3.23	55	4.1E-03	41	2.8E+01	-1.30
Cefadroxil	50370-12-2	1	39	-0.25	55	363.4	55	-2.96	55	2.8E-03	41	1.0E+01	-1.25
Cefetamet Pivoxil	65243-33-6	0.47	39	2.44	55	511.6	55	-5.31	55	3.9E-03	42	3.2E+03	-1.06
Cefixime	79350-37-1	0.6	39	-0.10	55	453.5	55	-3.82	55	1.8E-03	41	4.7E+01	-1.77
Celiprolol	56980-93-9	0.5	39	1.92	55	379.5	55	-3.13	55	1.1E-03	41	5.7E+00	1.16

Cephalexin	15686-71-2	0.96	39	0.35	55	347.4	55	-3.30	55	1.2E-02	41	9.2E+01	-1.61
Cephalothin	153-61-7	0	39	0.09	55	396.4	55	-3.47	55	1.5E-02	41	1.8E+02	-2.16
Cetirizine	83881-51-0	1	39	1.62	55	388.9	55	-2.17	55	2.6E-03	41	1.5E+00	1.43
Chlormezanone	80-77-3	1	39	0.48	55	273.7	55	-3.19	55	1.5E-03	41	9.1E+00	-0.48
Chlorothiazide	58-94-6	0.6	39	-0.15	55	295.7	55	-3.25	55	6.8E-03	41	4.8E+01	-1.83
Chloroxine	773-76-2	0.89	39	3.07	55	214.1	55	-3.34	55	1.9E-02	41	1.6E+02	0.85
Cicloprolol	94651-09-9	1	39	2.35	55	323.4	55	-2.47	55	1.5E-04	41	1.0E+00	2.35
Cidofovir	113852-37-2	0.03	39	-1.47	55	279.2	55	-1.09	55	1.1E-03	43	1.0E+00	-1.47
Cinolazepam	75696-02-5	0.95	39	2.24	55	357.8	55	-4.06	55	2.8E-05	41	1.3E+00	2.13
Ciprofloxacin	85721-33-1	0.69	39	1.63	55	331.3	55	-3.89	55	2.4E-03	41	7.4E+01	-0.24
Clenbuterol	37148-27-9	0.8	39	2.63	55	277.2	55	-2.80	55	2.2E-07	41	1.0E+00	2.63
Clomiphene	911-45-5	0.9	39	5.85	55	406.0	55	-5.48	55	2.5E-04	41	3.0E+02	3.37
Clopidogrel	113665-84-2	0.5	39	2.58	55	321.8	55	-3.52	55	2.3E-04	41	3.1E+00	2.09
Clorazepate	23887-31-2	0.91	39	2.54	55	314.7	55	-3.48	55	2.9E-04	43	3.5E+00	2.00
Colestipol	50925-79-6	0	39	-0.25	57	281.8	55	-1.42	57	1.1E-01	43	1.1E+01	-1.30
Cromolyn	16110-51-3	0.01	39	2.00	55	468.4	55	-5.41	55	1.7E-03	41	1.7E+03	-1.25
Cyclosporine A	59865-13-3	0.33	39	2.79	55	1202.6	55	-0.08	55	7.5E-04	43	1.0E+00	2.79

Cysteamine	60-23-1	0	39	0.22	55	77.2	55	0.04	55	2.6E-02	41	1.0E+00	0.22
Dapiprazole	72822-12-9	0	39	2.89	55	325.5	55	-4.17	55	7.7E-06	42	1.0E+00	2.89
Deferoxamine	70-51-9	0.02	39	-0.61	55	560.7	55	-2.47	55	1.1E-02	41	1.3E+01	-1.71
Delavirdine	136817-59-9	0.85	39	3.53	55	456.6	55	-3.12	55	8.8E-04	41	4.6E+00	2.87
Dextrose	50-99-7	0.99	39	-3.29	55	180.2	55	0.38	55	3.3E-02	41	1.0E+00	-3.29
Digitoxin	71-63-6	0.9	39	2.74	55	764.9	55	-4.44	55	1.6E-09	41	1.0E+00	2.74
Digoxin	20830-75-5	0.78	39	1.29	55	780.9	55	-4.09	55	7.7E-10	41	1.0E+00	1.29
Diphenoxylate	915-30-0	0.9	39	4.51	55	452.6	55	-5.21	55	4.4E-05	41	2.8E+01	3.06
Distigmine	17299-00-2	0.08	39	-5.15	57	416.5	55	-0.07	57	2.4E-05	42	1.0E+00	-5.15
Doxorubicin	23214-92-8	0.05	39	0.24	55	543.5	55	-4.52	55	2.7E-04	41	3.6E+01	-1.31
Droxidopa	23651-95-8	0.9	39	-1.86	55	213.2	55	0.67	55	8.4E-03	43	1.0E+00	-1.86
Emtricitabine	143491-57-0	0.93	39	-0.27	55	247.3	55	-2.24	55	9.7E-04	43	1.0E+00	-0.27
Enalapril	75847-73-3	0.63	39	3.25	55	376.5	55	-3.12	55	1.1E-04	41	1.0E+00	3.25
Enalaprilat	76420-72-9	0.1	39	3.63	55	348.4	55	-2.96	55	5.7E-05	43	1.0E+00	3.63
Entecavir	142217-69-4	1	39	-1.11	55	277.3	55	-2.39	55	3.6E-06	43	1.0E+00	-1.11
Ergoloid Mesylate	11032-41-0	0.25	39	2.62	57	631.7	55	-5.37	57	4.7E-06	43	4.5E+00	1.97
Erlotinib	183321-74-6	0.6	39	3.03	55	393.4	55	-4.80	55	7.6E-04	43	1.9E+02	0.75

Ertapenem	153832-46-3	0.9	39	-0.72	55	475.5	55	-2.80	55	2.1E-03	43	5.3E+00	-1.44
Estazolam	29975-16-4	0.93	39	2.52	55	294.7	55	-4.11	55	6.8E-06	41	1.0E+00	2.52
Ethosuximide	77-67-8	0.93	39	0.25	55	141.2	55	-0.54	55	7.1E-03	41	1.0E+00	0.25
Etofylline	519-37-9	0.8	39	-0.91	55	224.2	55	-0.15	55	2.2E-03	41	1.0E+00	-0.91
Etoposide	33419-42-0	0.5	39	0.28	55	588.6	55	-4.21	55	2.8E-04	41	1.8E+01	-0.97
Fenofibrate	49562-28-9	0.9	39	5.80	55	360.8	55	-5.52	55	5.5E-04	43	7.4E+02	2.93
Floxuridine	50-91-9	0.9	39	-1.41	55	246.2	55	-0.13	55	1.5E-04	41	1.0E+00	-1.41
Flunitrazepam	1622-62-4	0.8	39	2.13	55	313.3	55	-4.10	55	6.4E-06	41	1.0E+00	2.13
Fluocortolone	152-97-6	0.9	39	1.83	55	376.5	55	-3.77	55	2.7E-04	42	6.3E+00	1.04
Fluoxymesterone	76-43-7	0.44	39	2.27	55	336.4	55	-3.89	55	5.9E-05	43	1.8E+00	2.01
Folic Acid	59-30-3	0.75	39	-1.14	55	441.4	55	-2.89	55	1.8E-06	41	1.0E+00	-1.14
Fosinopril	98048-97-6	0.35	39	6.47	55	563.7	55	-4.92	55	1.4E-04	41	4.7E+01	4.79
Fructose	57-48-7	1	39	-1.03	55	180.2	55	-0.05	55	1.4E-01	41	1.0E+00	-1.03
Ganciclovir	82410-32-0	0.04	39	-1.61	55	255.2	55	-2.04	55	2.4E-03	43	1.0E+00	-1.62
Gemcitabine	95058-81-4	1	39	-2.22	55	263.2	55	-1.21	55	7.7E-03	43	1.0E+00	-2.22
Gitoxin	4562-36-1	0.95	39	1.60	55	780.9	55	-4.20	55	1.9E-06	50	1.0E+00	1.60
Glyceryl1Nitrate	624-43-1	0.89	39	-0.51	55	137.1	55	0.05	55	2.9E-04	41	1.0E+00	-0.51

Hydrocodone	125-29-1	0.8	39	2.57	55	299.4	55	-3.21	55	1.5E-04	41	1.0E+00	2.57
Hydroxyzine	68-88-2	0.8	39	2.32	55	374.9	55	-2.09	55	1.1E-03	41	1.0E+00	2.32
Imidapril	89371-37-9	0.7	39	2.28	55	405.4	55	-3.68	55	4.9E-05	43	1.0E+00	2.28
Indapamide	26807-65-8	0.9	39	1.96	55	365.8	55	-4.25	55	1.4E-05	43	1.0E+00	1.96
Indecainide	74517-78-5	1	39	3.87	55	308.4	55	-4.01	55	1.6E-03	42	6.7E+01	2.04
K-Strophanthoside	33279-57-1	0.16	39	-2.74	55	873.0	55	-3.07	55	2.9E-07	41	1.0E+00	-2.74
Leflunomide	75706-12-6	0.8	39	2.29	55	270.2	55	-3.77	55	7.4E-05	41	1.7E+00	2.05
Levodopa	59-92-7	0.86	39	-1.15	55	197.2	55	0.09	55	4.0E-02	41	1.0E+00	-1.15
Liothyronine	6893-02-3	0.95	39	3.91	55	651.0	55	-4.38	55	1.5E-07	41	1.0E+00	3.91
Lisinopril	76547-98-3	0.27	39	3.47	55	405.5	55	-2.96	55	9.9E-05	43	1.0E+00	3.47
Lofexidine	31036-80-3	0.9	39	3.04	55	259.1	55	-3.85	55	9.3E-06	41	1.0E+00	3.04
Lomustine	13010-47-4	1	39	2.72	55	233.7	55	-2.66	55	9.0E-04	41	1.6E+00	2.51
Loracarbef	76470-66-1	1	39	-1.60	55	349.8	55	-1.82	55	1.1E-03	41	1.0E+00	-1.60
Lymecycline	992-21-2	1	39	0.75	55	602.6	55	-3.82	55	6.8E-04	41	1.8E+01	-0.50
Mannitol	69-65-8	0.19	39	-3.26	55	182.2	55	0.43	55	3.3E-01	41	1.0E+00	-3.26
Mazindol	22232-71-9	0.93	39	2.36	55	284.7	55	-3.70	55	7.0E-06	41	1.0E+00	2.36
Memantine	19982-08-2	1	39	3.00	55	179.3	55	-2.68	55	1.1E-04	43	1.0E+00	3.00

Mepindolol	23694-81-7	0.82	39	2.30	55	262.4	55	-1.96	55	5.7E-05	42	1.0E+00	2.30
Mercaptopurine	50-44-2	0.5	39	-0.30	55	152.2	55	-2.17	55	9.9E-04	41	1.0E+00	-0.30
Methylphenobarbital	115-38-8	0.5	39	1.23	55	246.3	55	-2.40	55	2.4E-03	41	2.4E+00	0.84
Methylscopolamine	13265-10-6	0.175	39	-2.29	57	318.4	55	-0.17	57	9.4E-05	43	1.0E+00	-2.29
Midodrine	42794-76-3	0.93	39	-0.27	55	254.3	55	-0.47	55	5.9E-05	41	1.0E+00	-0.27
Miglitol	72432-03-2	1	39	-2.21	55	207.2	55	0.68	55	1.4E-03	41	1.0E+00	-2.21
Miglustat	72599-27-0	1	39	0.03	55	219.3	55	-0.19	55	1.4E-03	43	1.0E+00	0.03
Milnacipran	92623-85-3	0.84	39	0.83	55	246.4	55	-1.41	55	8.1E-04	43	1.0E+00	0.83
Minocycline	10118-90-8	1	39	2.12	55	457.5	55	-5.48	55	4.4E-04	43	5.3E+02	-0.60
Mitotane	53-19-0	0.4	39	5.41	55	320.0	55	-6.49	55	1.9E-02	43	2.3E+05	0.04
Mycophenolic Acid	24280-93-1	0.825	39	3.84	55	320.3	55	-3.77	55	2.2E-02	43	5.3E+02	1.11
N Acetylprocainamide	32795-44-1	0.83	39	1.51	55	277.4	55	-1.82	55	1.8E-03	41	1.0E+00	1.51
Nafarelin	76932-56-4	0	39	0.53	55	1322.5	55	-0.96	55	6.0E-07	43	1.0E+00	0.53
Nimodipine	66085-59-4	1	39	4.05	55	418.4	55	-4.96	55	8.6E-04	41	3.1E+02	1.55
Nitisinone	104206-65-7	0.9	39	0.99	55	329.2	55	-3.52	55	3.6E-04	43	4.9E+00	0.30
Norfenfluramine	1886-26-6	0.85	39	2.63	55	203.2	55	-2.33	55	9.8E-05	41	1.0E+00	2.63
Norfloxacin	70458-96-7	0.75	39	1.74	55	319.3	55	-3.35	55	2.5E-03	43	2.2E+01	0.40

Olanzapine	132539-06-1	1	39	3.08	55	312.4	55	-4.28	55	4.8E-05	41	3.7E+00	2.51
Ouabain	630-60-4	0.03	39	-2.21	55	584.7	55	-2.89	55	4.1E-05	41	1.0E+00	-2.21
Oxandrolone	53-39-4	0.97	39	3.39	55	306.4	55	-3.62	55	6.5E-05	41	1.1E+00	3.35
Oxtriphylline	4499-40-5	1	39	-2.41	57	283.3	55	0.10	57	2.1E-03	41	1.0E+00	-2.41
Pafenolol	75949-61-0	0.29	39	1.66	55	337.5	55	-4.96	55	3.0E-04	41	1.1E+02	-0.37
Palonosetron	135729-61-2	0.97	39	2.46	55	296.4	55	-3.32	55	8.4E-07	43	1.0E+00	2.46
Paromomycin	7542-37-2	0	39	-5.80	55	615.6	55	0.21	55	3.4E-03	41	1.0E+00	-5.80
Penicillin V	87-08-1	0.59	39	1.94	55	350.4	55	-2.85	55	4.3E-03	41	1.2E+01	0.85
Perhexiline	6621-47-2	0.8	39	6.47	55	277.5	55	-4.49	55	1.1E-03	41	1.4E+02	4.33
Phenacemide	63-98-9	1	39	0.87	55	178.2	55	-2.04	55	1.7E-02	41	7.3E+00	0.01
Phensuximide	86-34-0	1	39	0.04	55	189.2	55	-1.92	55	1.6E-02	41	5.3E+00	-0.69
Phenylalanine	150-30-1	1	39	0.24	55	165.2	55	-0.72	55	3.6E-02	41	1.0E+00	0.24
Phenylethylmalonamide	7206-76-0	0.91	39	0.35	55	206.2	55	-2.14	55	1.9E-03	41	1.1E+00	0.32
Pioglitazone	111025-46-8	0.83	39	3.50	55	356.4	55	-4.52	55	8.4E-05	43	1.1E+01	2.45
Pipemidic Acid	51940-44-4	0.93	39	-0.19	55	303.3	55	-2.06	55	2.6E-03	41	1.2E+00	-0.27
Piperacillin	61477-96-1	0	39	1.00	55	517.6	55	-4.41	55	4.6E-02	41	4.8E+03	-2.68
Pirazolac	71002-09-0	0.935	39	3.84	55	330.7	55	-4.70	55	1.8E-03	41	3.6E+02	1.28

Posaconazole	171228-49-2	0.96	39	4.67	55	700.8	55	-6.36	55	8.6E-04	43	7.8E+03	0.78
Pravastatin	81093-37-0	0.34	39	2.21	55	424.5	55	-3.85	55	9.4E-05	41	2.7E+00	1.78
Prednisone	53-03-2	0.95	39	1.57	55	358.4	55	-3.55	55	1.7E-04	43	2.4E+00	1.19
Pregabalin	148553-50-8	0.9	39	1.09	55	159.2	55	-0.89	55	2.8E-03	43	1.0E+00	1.09
Probucol	23288-49-5	0.07	39	9.00	55	516.8	55	-8.10	55	1.9E-03	42	9.7E+05	3.01
Procainamide	51-06-9	0.85	39	1.32	55	235.3	55	-1.60	55	1.3E-02	41	2.0E+00	1.01
Pyrimethamine	58-14-0	1	39	2.75	55	248.7	55	-3.77	55	3.0E-04	41	7.1E+00	1.90
Raloxifene	84449-90-1	0.6	39	4.57	55	473.6	55	-5.09	55	1.3E-03	41	6.2E+02	1.78
Ramelteon	196597-26-9	0.84	39	2.29	55	259.3	55	-3.51	55	3.1E-05	43	1.0E+00	2.29
Ranitidine	66357-35-5	0.57	39	-0.07	55	314.4	55	0.14	55	9.5E-04	43	1.0E+00	-0.07
Ribavirin	36791-04-5	0.85	39	-1.85	55	244.2	55	-1.66	55	4.9E-02	41	8.9E+00	-2.80
Rifampin	13292-46-1	0.8	39	2.05	55	822.9	55	-2.96	55	1.5E-03	41	5.3E+00	1.33
Rofecoxib	162011-90-7	0.93	39	-0.34	55	314.4	55	-2.52	55	1.6E-04	41	1.0E+00	-0.34
Rosiglitazone	122320-73-4	1	39	3.02	55	357.4	55	-4.38	55	2.2E-05	41	2.1E+00	2.70
Salicylic Acid	69-72-7	1	39	2.01	55	138.1	55	-1.36	55	1.8E-04	43	1.0E+00	2.01
Saquinavir	127779-20-8	0.3	39	5.08	55	670.8	55	-5.48	55	3.0E-03	43	3.6E+03	1.52
Spironolactone	52-01-7	0.73	39	3.15	55	416.6	55	-5.28	55	9.6E-04	43	7.4E+02	0.28

Sulfadiazine	68-35-9	0.93	39	-0.07	55	250.3	55	-2.49	55	1.6E-02	43	2.0E+01	-1.37
Sulfamerazine	127-79-7	0.81	39	0.11	55	264.3	55	-2.72	55	1.5E-02	41	3.2E+01	-1.40
Sulfapyridine	144-83-2	0.7	39	0.47	55	249.3	55	-2.51	55	2.4E-02	42	3.1E+01	-1.02
Teicoplanin A2 1	91032-34-7	0	39	1.51	55	1877.6	55	-10.62	55	2.1E-04	43	3.6E+07	-6.04
Temozolomide	85622-93-1	1	39	-1.27	55	194.2	55	-1.89	55	1.7E-03	43	1.0E+00	-1.27
Tetracycline	60-54-8	0.8	39	0.62	55	444.4	55	-4.31	55	4.5E-03	41	3.7E+02	-1.95
Theophylline	58-55-9	1	39	-0.28	55	180.2	55	-1.14	55	2.9E-03	41	1.0E+00	-0.28
Thioridazine	50-52-2	0.6	39	5.90	55	370.6	55	-6.15	55	2.2E-03	41	1.2E+04	1.81
Toliprolol	2933-94-0	0.9	39	1.80	55	223.3	55	-1.42	55	1.3E-03	48	1.0E+00	1.80
Treosulfan	299-75-2	0.97	39	-0.77	55	278.3	55	-1.89	55	3.9E-03	42	1.2E+00	-0.84
Trimethobenzamide	138-56-7	0.8	39	1.26	55	388.5	55	-2.48	55	2.6E-03	41	3.1E+00	0.77
Valdecoxib	181695-72-7	0.83	39	3.57	55	314.4	55	-4.33	55	1.3E-04	42	1.1E+01	2.53
Verapamil	52-53-9	0.95	39	4.02	55	454.6	55	-4.80	55	1.1E-03	43	2.6E+02	1.60
Vidarabine	5536-17-4	0	39	-0.76	55	267.2	55	-1.60	55	6.7E-03	42	1.1E+00	-0.79
Vigabatrin	60643-86-9	1	39	-0.30	55	129.2	55	0.10	55	2.3E-02	43	1.0E+00	-0.30
Vitamin E	59-02-9	0.65	39	10.96	55	430.7	55	-7.92	55	7.0E-04	42	2.3E+05	5.60
Voriconazole	137234-62-9	0.96	39	1.21	55	349.3	55	-3.92	55	1.1E-03	43	3.8E+01	-0.38

Warfarin	81-81-2	0.97	39	3.13	55	308.3	55	-4.20	55	3.2E-05	41	2.1E+00	2.81
Xamoterol	81801-12-9	0.07	39	-0.70	55	339.4	55	-1.96	55	1.2E-03	43	1.0E+00	-0.70
Zidovudine	30516-87-1	0.97	39	-0.53	57	267.2	55	-1.32	57	2.2E-03	41	1.0E+00	-0.53
Abiraterone Acetate	154229-18-2	0.45	39	6.58	55	391.6	55	-6.17	55	2.6E-03	43	1.5E+04	2.40
Gemifloxacin	175463-14-6	0.6	39	1.77	55	389.4	55	-3.85	55	8.2E-04	43	2.3E+01	0.40
Altretamine	645-05-6	0.87	39	2.53	55	210.3	55	-2.80	55	1.5E-03	41	3.9E+00	1.95
Alogliptin	850649-61-5	1	39	1.62	55	339.4	55	-4.00	55	7.4E-05	43	3.0E+00	1.15
Lercanidipine	100427-26-7	0.44	39	7.56	55	611.7	55	-7.25	55	4.9E-05	42	3.5E+03	4.02
Lorcaserin Hydrochloride	616202-92-7	0.92	39	2.96	55	195.7	55	-2.30	55	1.0E-04	43	1.0E+00	2.96
Candoxatril	118785-03-8	0.38	39	3.28	55	515.6	55	-4.74	55	3.9E-04	41	8.6E+01	1.34
Delapril	83435-66-9	0.45	39	4.48	55	452.5	55	-4.00	55	2.7E-04	42	1.1E+01	3.45
Ezogabine	150812-12-7	0.84	39	0.96	55	303.3	55	-3.82	55	4.0E-03	43	1.1E+02	-1.07
Mycophenolate Mofetil	128794-94-5	0.963	39	3.69	55	433.5	55	-3.66	55	1.7E-02	41	3.0E+02	1.21
Enoxacin	74011-58-8	0.89	39	1.59	55	320.3	55	-2.72	55	3.7E-03	41	7.9E+00	0.69
Cilostazol	73963-72-1	0.74	39	3.36	55	369.5	55	-5.04	55	5.4E-04	43	2.4E+02	0.98
Loxoprofen	68767-14-6	0.58	39	1.69	55	246.3	55	-2.82	55	7.3E-04	43	1.9E+00	1.40
Eltrombopag Olamine	496775-61-2	0.52	39	4.71	55	442.5	55	-5.32	55	3.4E-04	43	2.8E+02	2.26

Valacyclovir	124832-26-4	0.36	39	-0.45	55	324.3	55	-3.18	55	9.2E-03	41	5.6E+01	-2.20
Vilazodone	163521-12-8	0.98	39	3.98	57	441.5	55	-6.33	57	9.1E-05	43	7.7E+02	1.09
Febuxostat	144060-53-7	0.89	39	4.00	55	316.4	55	-4.96	55	3.8E-04	43	1.4E+02	1.86
Vismodegib	879085-55-9	0.693	39	2.03	55	421.3	55	-5.51	55	3.6E-04	43	4.6E+02	-0.63
UK-294,315	192868-49-8	0.86	39	2.50	55	509.6	55	-4.52	55	7.8E-05	45	1.0E+01	1.48
Spirapril	83647-97-6	0.6	39	5.88	55	466.6	55	-4.34	55	5.1E-05	42	4.5E+00	5.23
Vildagliptin	274901-16-5	0.85	39	0.17	55	303.4	55	-2.00	55	3.3E-04	42	1.0E+00	0.17
Levothyroxine	51-48-9	0.6	39	4.72	55	776.9	55	-5.00	55	6.4E-07	41	1.0E+00	4.72
Lacosamide	175481-36-4	1	39	0.73	55	250.3	55	-1.36	55	1.6E-03	43	1.0E+00	0.73
Carglumic Acid	1188-38-1	0.4	39	-0.74	55	190.2	55	-0.92	55	7.9E-02	43	2.6E+00	-1.16
Nelfinavir	159989-64-7	0.78	39	7.28	55	567.8	55	-5.82	55	4.4E-03	43	1.2E+04	3.21
Saxagliptin	361442-04-8	0.75	39	0.20	55	315.4	55	-2.96	55	1.6E-05	43	1.0E+00	0.20
Fidaxomicin	873857-62-6	0.08	39	9.14	55	1058.0	55	-5.52	55	3.8E-04	43	5.0E+02	6.43
Orlistat	96829-58-2	0.17	39	7.00	55	495.7	55	-7.32	55	7.3E-04	41	6.1E+04	2.22
Atazanavir sulfate	198904-31-3	0.8	39	3.89	55	704.9	55	-4.82	55	5.7E-04	43	1.5E+02	1.71
Levocetirizine dihydrochloride	130018-77-8	0.854	39	1.62	55	388.9	55	-2.17	55	1.3E-05	43	1.0E+00	1.62
Sertraline	79617-96-2	0.86	39	5.08	55	306.2	55	-4.77	55	6.5E-04	41	1.5E+02	2.89

Sirolimus	53123-88-9	0.9	39	4.26	55	914.2	55	-3.57	55	8.9E-06	41	1.0E+00	4.26
Hydromorphone	466-99-9	0.87	39	2.13	55	285.3	55	-2.74	55	8.4E-05	41	1.0E+00	2.13
Lenalidomide	191732-72-6	0.9	39	-1.47	55	259.3	55	-1.17	55	9.6E-05	43	1.0E+00	-1.47
Crizotinib	877399-52-5	0.47	39	3.55	55	450.3	55	-5.57	55	1.1E-03	43	1.6E+03	0.33
Enzalutamide	915087-33-1	0.85	39	2.98	55	464.4	55	-5.82	55	3.4E-04	43	9.2E+02	0.02
Pomalidomide	19171-19-8	0.83	39	-0.71	55	273.2	55	-2.11	55	1.5E-05	43	1.0E+00	-0.71
Canagliflozin	842133-18-0	0.84	39	2.71	55	444.5	55	-5.23	55	6.7E-04	43	4.6E+02	0.05
Etravirine	269055-15-4	0.16	39	3.88	55	435.3	55	-7.27	55	9.2E-04	43	6.8E+04	-0.96
Rilpivirine	500287-72-9	0.75	39	4.53	55	366.4	55	-6.59	55	6.8E-05	43	1.0E+03	1.51
Indacaterol maleate	312753-06-3	0.45	39	4.09	55	392.5	55	-4.64	55	7.6E-07	43	1.0E+00	4.09
Boceprevir	394730-60-0	0.92	39	2.84	55	519.7	55	-4.52	55	4.6E-03	43	6.2E+02	0.05
Lopinavir	192725-17-0	0.807	39	5.42	55	628.8	55	-6.24	55	1.3E-03	43	8.9E+03	1.47
Cinacalcet	226256-56-0	0.8	39	6.19	55	357.4	55	-5.77	55	1.0E-03	43	2.4E+03	2.81
Ceftibuten	97519-39-6	0.7	39	-3.19	55	410.4	55	-2.10	55	9.7E-04	43	1.0E+00	-3.19
Fomepizole	7554-65-6	1	39	1.10	55	82.1	55	-1.37	55	2.2E-02	43	2.0E+00	0.79
Varenicline tartrate	249296-44-4	0.92	39	1.01	55	211.3	55	-2.03	55	9.5E-06	43	1.0E+00	1.01
Desvenlafaxine Succinate	93413-62-8	0.805	39	1.74	55	263.4	55	-1.57	55	1.9E-04	43	1.0E+00	1.74

Ezetimibe	163222-33-1	0.31	39	3.96	55	409.4	55	-5.37	55	2.4E-05	43	2.3E+01	2.60
Celecoxib	169590-42-5	0.97	39	2.59	55	381.4	55	-4.43	55	1.0E-03	41	1.1E+02	0.54
Rufinamide	106308-44-5	0.85	39	1.00	55	238.2	55	-2.77	55	1.3E-02	43	3.2E+01	-0.50
Dalfampridine	504-24-5	1	39	0.34	55	94.1	55	-0.32	55	2.1E-04	43	1.0E+00	0.34
Temocapril	111902-57-9	0.6	39	6.57	55	476.6	55	-5.46	55	8.4E-06	43	9.6E+00	5.59
Amprenavir	161814-49-9	0.89	39	2.68	55	505.6	55	-4.72	55	5.5E-03	43	1.2E+03	-0.39
Ephedrine	299-42-3	0.97	39	1.08	55	165.2	55	-0.66	55	6.1E-04	41	1.0E+00	1.08
Ruxolitinib	941678-49-5	0.95	39	2.07	55	306.4	55	-4.74	55	1.6E-04	43	3.6E+01	0.51
Darifenacin hydrobromide	133099-04-4	0.79	39	3.78	55	426.6	55	-5.60	55	3.5E-05	43	5.6E+01	2.03
Gabapentin	60142-96-3	0.74	39	1.08	55	171.2	55	-0.80	55	7.0E-03	41	1.0E+00	1.08
Azosemide	27589-33-9	0.2	39	1.40	55	370.8	55	-4.40	55	3.2E-04	43	3.2E+01	-0.11
Ticagrelor	274693-27-5	0.73	39	2.02	55	522.6	55	-5.02	55	3.4E-04	43	1.5E+02	-0.15
Tapentadol	175591-23-8	0.99	39	3.02	55	221.3	55	-2.36	55	2.7E-03	43	2.5E+00	2.63
Acenocoumarol	152-72-7	0.9	39	2.97	55	353.3	55	-4.77	55	3.4E-05	41	8.0E+00	2.07
Azathioprine	446-86-6	0.87	39	-1.05	55	277.3	55	-2.52	55	1.1E-03	41	1.4E+00	-1.21
Calcitriol	32222-06-3	1	39	5.63	55	416.6	55	-5.62	55	7.2E-09	41	1.0E+00	5.63
Cefprozil	92665-29-7	0.95	39	-0.60	55	389.4	55	-2.80	55	2.6E-03	41	6.4E+00	-1.41

Chenodeoxycholic Acid	474-25-9	1	39	4.76	55	392.6	55	-5.29	55	6.4E-04	41	5.0E+02	2.06
Diethylcarbamazine	90-89-1	0.9	39	1.66	55	199.3	55	-1.96	55	1.8E-03	41	1.0E+00	1.66
Formoterol	73573-87-2	0.65	39	2.03	55	344.4	55	-3.42	55	4.7E-04	41	4.9E+00	1.34
Lodoxamide Trometamol	53882-12-5	0.7	39	-0.38	55	311.6	55	-3.46	55	3.2E-06	43	1.0E+00	-0.38
Loperamide Hydrochloride	53179-11-6	0.76	39	4.15	55	477.0	55	-3.96	55	3.4E-05	43	1.2E+00	4.06
Octreotide	83150-76-9	0.05	39	3.40	55	1019.2	55	-5.37	55	1.5E-06	43	1.4E+00	3.26
Pergolide	66104-22-1	0.6	39	3.90	55	314.5	55	-3.70	55	9.5E-06	41	1.0E+00	3.90
Pirenzepine	28797-61-7	0.2	39	0.21	55	351.4	55	-2.49	55	4.3E-04	41	1.0E+00	0.21
Terlipressin	14636-12-5	0.05	39	-3.32	55	1227.4	55	-2.30	55	9.8E-06	43	1.0E+00	-3.32
Ursodiol	128-13-2	1	39	4.76	55	392.6	55	-5.29	55	1.5E-03	41	1.2E+03	1.68
Xipamide	14293-44-8	0.8	39	2.19	55	354.8	55	-4.74	55	1.1E-04	41	2.5E+01	0.79
Olopatadine	113806-05-6	0.7	39	2.96	55	337.4	55	-3.64	55	5.9E-05	41	1.0E+00	2.95
Adinazolam	37115-32-5	1	39	1.27	55	351.8	55	-3.49	55	8.5E-05	41	1.1E+00	1.24
Alfentanil	71195-58-9	1	39	2.16	55	416.5	55	-3.77	55	3.5E-05	41	1.0E+00	2.16
Alizapride	59338-93-1	1	39	0.84	55	315.4	55	-1.24	55	1.9E-03	42	1.0E+00	0.84
Amiodarone	1951-25-3	1	39	7.82	55	645.3	55	-7.12	55	2.5E-03	41	1.3E+05	2.70
Amisulpride	71675-85-9	1	39	1.50	55	369.5	55	-2.64	55	3.2E-03	42	5.6E+00	0.74

Amlodipine	88150-42-9	0.95	39	3.01	55	408.9	55	-4.36	55	2.5E-05	41	2.2E+00	2.66
Atomoxetine	83015-26-3	1	39	3.36	55	255.4	55	-3.14	55	3.9E-04	43	2.1E+00	3.03
Atovaquone	95233-18-4	0.06	39	6.47	55	366.8	55	-7.66	55	6.1E-03	41	1.1E+06	0.42
Azithromycin	83905-01-5	0.6	39	2.58	55	749.0	55	-0.59	55	1.3E-03	43	1.0E+00	2.58
Bromfenac	91714-94-2	1	39	2.02	55	334.2	55	-3.52	55	3.6E-07	43	1.0E+00	2.02
Buflomedil	55837-25-7	1	39	3.13	55	307.4	55	-3.03	55	2.0E-03	41	8.3E+00	2.21
Bufuralol	54340-62-4	1	39	3.54	55	261.4	55	-3.21	55	2.3E-04	41	1.5E+00	3.37
Bupivacaine	38396-39-3	0.9	39	3.31	55	288.4	55	-3.07	55	7.8E-04	41	3.7E+00	2.75
Cefazolin	25953-19-9	1	39	-0.70	55	454.5	55	-4.41	55	8.8E-03	41	9.0E+02	-3.65
Cefcanel	41952-52-7	0.42	39	0.16	55	478.6	55	-4.10	55	6.3E-04	46	3.1E+01	-1.34
Cefetamet	65052-63-3	0.52	39	-0.24	55	397.4	55	-3.62	55	5.0E-03	42	8.4E+01	-2.16
Cerivastatin	145599-86-6	1	39	3.18	55	459.6	55	-4.07	55	6.5E-07	41	1.0E+00	3.18
Cibenzoline	53267-01-9	1	39	3.49	55	262.4	55	-4.15	55	7.6E-04	41	4.3E+01	1.86
Clarithromycin	81103-11-9	1	39	2.81	55	748.0	55	-1.11	55	6.7E-04	41	1.0E+00	2.81
Clinafloxacin	105956-97-6	1	39	2.45	55	365.8	55	-5.04	55	1.1E-03	42	4.8E+02	-0.23
Cloxacillin	61-72-3	0.75	39	2.83	55	435.9	55	-4.18	55	4.6E-03	41	2.8E+02	0.38
Conivaptan	210101-16-9	1	39	5.42	55	498.6	55	-6.70	55	8.0E-05	43	1.6E+03	2.21

Cyclophosphamide	50-18-0	0.825	39	0.73	55	261.1	55	-0.80	55	1.1E-03	41	1.0E+00	0.73
Dexloxiglumide	119817-90-2	0.95	39	4.37	55	461.4	55	-4.01	55	4.3E-04	41	1.8E+01	3.12
Dicloxacillin	3116-76-5	1	39	3.10	55	470.3	55	-4.77	55	2.1E-03	41	5.0E+02	0.40
Didanosine	69655-05-6	0.5	39	-1.43	55	236.2	55	-1.64	55	1.7E-03	41	1.0E+00	-1.43
Dyphylline	479-18-5	0.95	39	-1.25	55	254.2	55	-0.26	55	1.4E-02	41	1.0E+00	-1.25
Doxapram	309-29-5	1	39	5.64	55	378.5	55	-4.41	55	6.3E-04	41	6.5E+01	3.83
Doxifluridine	3094-09-5	0.9	39	-0.72	55	246.2	55	-0.34	55	4.9E-03	41	1.0E+00	-0.72
Doxycycline	564-25-0	1	39	1.78	55	444.4	55	-4.89	55	4.5E-04	43	1.4E+02	-0.36
Drotaverine	14009-24-6	1	39	3.91	55	397.5	55	-4.77	55	6.0E-04	42	1.4E+02	1.75
Encainide	66778-36-7	0.95	39	3.75	55	352.5	55	-4.59	55	5.7E-04	41	8.7E+01	1.81
Entacapone	130929-57-6	0.5	39	2.12	55	305.3	55	-2.13	55	5.2E-03	43	2.8E+00	1.66
Epristeride	119169-78-7	0.93	39	5.71	55	399.6	55	-5.96	55	1.3E-05	41	4.6E+01	4.05
Eprosartan	133040-01-4	0.15	39	2.96	55	424.5	55	-5.31	55	1.9E-03	41	1.5E+03	-0.23
Etilefrine	709-55-7	1	39	0.63	55	181.2	55	-0.32	55	2.8E-04	41	1.0E+00	0.63
Fenspiride	5053-06-5	1	39	0.89	55	260.3	55	-2.54	55	1.8E-03	41	2.5E+00	0.49
Fleroxacin	79660-72-3	1	39	1.84	55	369.3	55	-3.96	55	1.1E-03	42	3.9E+01	0.24
Flupirtine	56995-20-1	1	39	1.60	55	304.3	55	-3.49	55	2.0E-03	42	2.5E+01	0.21

Frovatriptan	158747-02-5	0.4	39	0.93	55	243.3	55	-2.15	55	3.1E-05	41	1.0E+00	0.93
Ginkgolide A	15291-75-5	0.9	39	-0.04	55	408.4	55	-1.82	55	8.8E-06	46	1.0E+00	-0.04
Ginkgolide B	15291-77-7	0.9	39	2.07	55	424.4	55	-2.64	55	8.5E-06	47	1.0E+00	2.07
Hydroxyurea	127-07-1	1	39	-1.80	55	76.1	55	1.11	55	2.8E-02	43	1.0E+00	-1.80
Idazoxan	79944-58-4	0.95	39	2.31	55	204.2	55	-3.11	55	2.0E-04	41	1.0E+00	2.30
Ifosfamide	3778-73-2	1	39	0.76	55	261.1	55	-0.80	55	7.7E-03	43	1.0E+00	0.76
Levofloxacin	100986-85-4	1	39	1.86	55	361.4	55	-3.72	55	2.1E-03	43	4.4E+01	0.21
Levomepromazine	60-99-1	0.53	39	4.94	55	328.5	55	-5.19	55	6.1E-04	41	3.7E+02	2.37
Levoprotiline	76496-68-9	1	39	3.13	55	293.4	55	-3.41	55	1.7E-04	41	1.7E+00	2.89
Lorcainide	59729-31-6	0.7	39	3.62	55	370.9	55	-3.85	55	1.1E-03	41	3.1E+01	2.14
Lovastatin	75330-75-5	0.31	39	4.31	55	404.5	55	-4.70	55	2.0E-04	41	3.9E+01	2.72
Loxiglumide	107097-80-3	1	39	4.37	55	461.4	55	-4.01	55	1.7E-03	41	7.2E+01	2.51
Melagatran	159776-70-2	0.15	39	2.42	55	473.6	55	-4.35	55	6.3E-06	41	1.0E+00	2.42
Methotrexate	59-05-2	0.7	39	-0.45	55	454.4	55	-4.21	55	6.6E-05	41	4.3E+00	-1.08
Mirtazapine	61337-67-5	0.8	39	0.89	55	265.4	55	-2.37	55	1.7E-04	41	1.0E+00	0.89
Montelukast	158966-92-8	0.8	39	5.81	55	586.2	55	-7.44	55	1.7E-05	41	1.9E+03	2.53
Nevirapine	129618-40-2	1	39	2.64	55	266.3	55	-3.14	55	1.5E-03	43	8.2E+00	1.72

Nomifensine	24526-64-5	1	39	1.01	55	238.3	55	-2.15	55	8.4E-04	41	1.0E+00	1.01
Oseltamivir Acid	187227-45-8	0.8	39	0.74	55	284.4	55	-1.59	55	1.1E-03	42	1.0E+00	0.74
Oxiracetam	62613-82-5	0.75	39	-2.48	55	158.2	55	0.62	55	5.1E-03	41	1.0E+00	-2.48
Paricalcitol	131918-61-1	0.861	39	5.90	55	416.6	55	-5.74	55	3.5E-08	43	1.0E+00	5.90
Penciclovir	39809-25-1	0.1	39	-1.35	55	253.3	55	-1.92	55	3.9E-05	43	1.0E+00	-1.35
Phencyclidine	77-10-1	0.95	39	4.25	55	243.4	55	-3.09	55	4.9E-05	41	1.0E+00	4.25
Physostigmine	57-47-6	0.05	39	1.27	55	275.4	55	-1.52	55	3.6E-06	41	1.0E+00	1.27
Pirmenol	68252-19-7	0.95	39	3.57	55	338.5	55	-2.89	55	4.4E-04	41	1.4E+00	3.43
Pyridostigmine	155-97-5	0.1	39	-4.31	57	181.2	55	0.39	57	6.6E-03	41	1.0E+00	-4.31
Quinaprilat	82768-85-2	0.61	39	5.18	55	410.5	55	-4.20	55	9.7E-05	43	6.2E+00	4.38
Reboxetine	71620-89-8	1	39	2.45	55	313.4	55	-2.96	55	3.8E-05	43	1.0E+00	2.45
Rifabutin	72559-06-9	0.53	39	4.49	55	847.0	55	-4.48	55	7.1E-04	42	8.6E+01	2.56
Ritonavir	155213-67-5	0.7	39	2.33	55	720.9	55	-4.57	55	1.7E-03	43	2.5E+02	-0.06
Roquinimex	84088-42-6	1	39	1.03	55	308.3	55	-2.20	55	1.6E-05	41	1.0E+00	1.03
Rosuvastatin	287714-41-4	0.5	39	0.89	55	481.5	55	-3.44	55	8.3E-05	43	1.0E+00	0.89
Sematilide	101526-83-4	0.65	39	1.44	55	313.4	55	-1.60	55	3.2E-04	41	1.0E+00	1.44
Sildenafil	139755-83-2	0.92	39	2.47	55	474.6	55	-4.96	55	2.1E-04	41	7.7E+01	0.58

Sitafloxacin	127254-12-0	0.95	39	2.62	55	409.8	55	-5.25	55	6.1E-04	41	4.4E+02	-0.02
Sitagliptin	486460-32-6	0.95	39	2.06	55	407.3	55	-4.82	55	2.5E-04	43	6.5E+01	0.24
Solifenacin	242478-37-1	1	39	4.16	55	362.5	55	-4.55	55	2.8E-05	43	3.9E+00	3.56
Sufentanil	56030-54-7	0.9	39	3.95	55	386.6	55	-3.42	55	3.9E-06	41	1.0E+00	3.95
Suprofen	40828-46-4	0.92	39	2.18	55	260.3	55	-3.34	55	3.1E-03	42	2.7E+01	0.76
Suramin	145-63-1	0	39	-6.24	55	1297.3	55	-3.66	55	7.7E-04	43	1.4E+01	-7.38
Tacrolimus	104987-11-3	0.15	39	4.79	55	804.0	55	-4.64	55	2.0E-05	42	3.5E+00	4.24
Talinolol	38649-73-9	0.65	39	2.98	55	363.5	55	-3.80	55	8.3E-04	42	2.1E+01	1.66
Tegaserod	145158-71-0	0.5	39	3.22	55	301.4	55	-3.96	55	4.0E-05	43	1.4E+00	3.06
Cefoperazone	62893-19-0	0.1	40	-1.11	55	645.7	55	-4.24	55	1.9E-02	41	1.3E+03	-4.22
Terodiline	15793-40-5	1	39	4.68	55	281.4	55	-4.12	55	1.8E-04	43	9.4E+00	3.71
Cefoxitin	35607-66-0	0.15	40	0.00	55	427.5	55	-3.85	55	2.8E-02	41	8.0E+02	-2.90
Tizanidine	51322-75-9	1	39	2.39	55	253.7	55	-3.92	55	1.4E-04	41	4.7E+00	1.71
Griseofulvin	126-07-8	0.43	40	2.01	55	352.8	55	-3.96	55	2.1E-03	41	7.7E+01	0.13
Nordazepam	1088-11-5	0.99	40	2.78	55	270.7	55	-3.55	55	3.7E-05	3	1.0E+00	2.78
Vardenafil	224785-90-4	0.9	39	3.64	55	488.6	55	-5.59	55	4.1E-05	43	6.3E+01	1.84
Promazine	58-40-2	1	40	4.69	55	284.4	55	-4.82	55	3.5E-03	41	9.4E+02	1.72

Vinblastine	865-21-4	0.05	39	5.92	55	811.0	55	-4.37	55	3.7E-05	43	3.4E+00	5.39
Thiacetazone	104-06-3	0.2	40	1.49	55	236.3	55	-3.39	55	6.3E-04	41	6.2E+00	0.69
Zolmitriptan	139264-17-8	0.915	39	0.46	55	287.4	55	-2.70	55	3.5E-05	43	1.0E+00	0.46
Viomycin	32988-50-4	0.85	3	-4.33	55	685.7	55	-2.15	55	5.8E-03	41	3.3E+00	-4.85
Deferasirox	201530-41-8	0.81	39	5.15	55	373.4	55	-5.32	55	6.4E-03	43	5.4E+03	1.42
Cytarabine	147-94-4	0.2	19	-1.81	55	243.2	55	-6.33	55	6.7E-04	41	5.7E+03	-5.56
Maraviroc	376348-65-1	0.75	39	5.30	55	513.7	55	-6.33	55	1.2E-03	43	9.9E+03	1.31
Erythritol	149-32-6	0.9	19	-2.17	55	122.1	55	0.73	55	8.2E-04	42	1.0E+00	-2.17
Bosentan	147536-97-8	0.698	39	4.36	55	551.6	55	-6.00	55	4.5E-04	43	1.8E+03	1.10
Rivaroxaban	366789-02-8	0.66	39	1.71	55	435.9	55	-4.74	55	6.9E-05	43	1.5E+01	0.52
Cefamandole	34444-01-4	0	39	-0.04	55	462.5	55	-4.12	55	1.3E-02	41	6.9E+02	-2.88
Ceforanide	60925-61-3	0	39	-0.36	55	519.6	55	-4.11	55	3.8E-03	41	2.0E+02	-2.66
Pranlukast	103177-37-3	0.2	39	4.05	55	481.5	55	-5.85	55	1.9E-03	42	5.3E+03	0.33
Penicillin G	61-33-6	0.3	39	1.92	55	334.4	55	-2.89	55	3.6E-02	43	1.1E+02	-0.12

Table A.2 Physical Properties, Dose, Fraction absorbed, calculated absorption parameter Π^{MP}, and calculated maximum well-absorbed dose for Drugs used in Chapter 4

Name	CAS NO	FA	Melting Point	Ref for MP	log P	log S	Dose D in mole	Check	Π^{MP}	Calculated Dose
Abacavir	136470-78-5	0.83	165	73	1.16	-4.10	2.10E-03	suspension	1.18	3.15E-02
Abiraterone Acetate	154229-18-2	0.45	147	73	6.58	-6.17	2.55E-03	suspension	1.27	4.76E-02
Acebutolol	37517-30-9	0.85	121	73	1.77	-2.40	3.57E-03	suspension	1.39	8.67E-02
Acenocoumarol	152-72-7	0.90	197.5	73	2.97	-4.77	3.40E-05	suspension	2.64	1.49E-02
Acetazolamide	59-66-5	1.00	258.5	73	-0.26	-1.89	4.51E-03	suspension	-0.09	3.66E-03
Acetohexamide	968-81-0	0.80	166	73	2.44	-3.62	4.62E-03	suspension	0.82	3.08E-02
Acitretin	55079-83-9	0.95	229	73	6.00	-4.89	2.30E-04	suspension	1.50	7.21E-03
Acyclovir	59277-89-3	0.23	256.7	73	-1.48	-1.85	3.54E-03	suspension	0.03	3.81E-03
Adinazolam	37115-32-5	1.00	171.7	73	1.27	-3.49	8.53E-05	suspension	2.50	2.70E-02
Albendazole	54965-21-8	0.05	209	73	3.00	-4.57	3.01E-03	suspension	0.58	1.14E-02
Alfacalcidol	41294-56-8	1.00	135	73	7.64	-6.25	4.49E-07	suspension	5.15	6.28E-02

Allopurinol	315-30-0	0.80	380	73	-0.55	-2.77	5.86E-03	suspension	-1.42	2.23E-04
Almitrine	27469-53-0	0.90	181	73	6.11	-6.59	2.09E-04	suspension	2.02	2.18E-02
Almotriptan	154323-57-6	0.75	109.5	211	2.30	-3.89	7.45E-05	suspension	3.18	1.13E-01
Alogliptin	850649-61-5	1.00	127.5	103	1.62	-4.00	7.37E-05	suspension	3.01	7.46E-02
Alprenolol	13655-52-2	0.93	64.5	189	2.91	-2.10	3.21E-03	suspension	2.00	3.18E-01
Altretamine	645-05-6	0.87	173	73	2.53	-2.80	1.54E-03	suspension	1.23	2.62E-02
Amantadine	768-94-5	0.90	186	73	2.44	-2.42	2.65E-03	suspension	0.87	1.94E-02
Amdinocillin	32887-01-7	0.05	156	73	2.33	-3.74	2.77E-03	suspension	1.15	3.87E-02
Aminoglutethimide	125-84-8	1.00	149.5	73	0.54	-1.85	4.31E-03	suspension	1.02	4.50E-02
Amisulpride	71675-85-9	1.00	126.5	73	1.50	-2.64	3.25E-03	suspension	1.37	7.64E-02
Amitriptyline	50-48-6	0.95	196.5	202	4.41	-3.92	1.08E-03	suspension	1.15	1.52E-02
Amlodipine	88150-42-9	0.95	135.5	101	3.01	-4.36	2.45E-05	suspension	3.40	6.21E-02
Amobarbital	57-43-2	0.95	157	73	2.18	-2.68	4.42E-03	suspension	0.93	3.78E-02
Amoxapine	14028-44-5	0.95	175.5	73	2.93	-4.23	1.91E-03	suspension	1.11	2.47E-02
Amoxicillin	26787-78-0	0.92	194	204	0.88	-1.96	4.11E-03	suspension	0.59	1.61E-02
Ampicillin	69-53-4	0.62	201.5	73	1.48	-2.33	1.00E-02	suspension	0.13	1.36E-02
Amprenavir	161814-49-9	0.89	73	167	2.68	-4.72	5.54E-03	suspension	1.67	2.62E-01

Anagrelide	68475-42-3	0.70	300	83	2.13	-3.82	3.90E-05	suspension	1.56	1.41E-03
Antrafenine	55300-29-3	1.00	88	73	6.22	-6.20	5.10E-04	suspension	2.56	1.85E-01
Apricitabine	160707-69-7	0.80	200	73	-0.21	-2.11	3.49E-03	suspension	0.61	1.41E-02
Aripiprazole	129722-12-9	0.87	139.2	73	3.76	-3.74	6.69E-05	suspension	2.93	5.70E-02
Aspirin	50-78-2	0.82	135	73	1.40	-1.96	2.22E-02	suspension	0.45	6.28E-02
Astemizole	68844-77-9	1.00	172.9	73	5.52	-6.16	2.19E-05	suspension	3.08	2.62E-02
Atazanavir sulfate	198904-31-3	0.80	208	73	3.89	-4.82	5.67E-04	suspension	1.31	1.17E-02
Atovaquone	95233-18-4	0.06	217.5	73	6.47	-7.66	6.13E-03	suspension	0.19	9.40E-03
Azathioprine	446-86-6	0.87	243.5	73	-1.05	-2.52	1.08E-03	suspension	0.68	5.16E-03
Azelastine	58581-89-8	1.00	25	73	3.47	-4.72	2.09E-05	suspension	4.58	7.91E-01
Azlocillin	37091-66-0	0.00	163.5	190	0.83	-4.14	1.30E-02	suspension	0.40	3.26E-02
Azosemide	27589-33-9	0.20	219.5	73	1.40	-4.40	3.24E-04	suspension	1.44	8.97E-03
Aztreonam	78110-38-0	0.01	227	73	0.49	-4.07	1.83E-02	suspension	-0.39	7.55E-03
Benazepril	86541-75-5	0.50	148.5	73	4.54	-4.00	1.88E-04	suspension	2.39	4.60E-02
Bendroflumethiazide	73-48-3	1.00	225	73	1.29	-3.96	4.74E-05	suspension	2.22	7.91E-03
Benorylate	5003-48-5	1.00	175.5	73	2.15	-4.57	2.55E-02	suspension	-0.01	2.47E-02
Benzbromarone	3562-84-3	0.73	151	73	6.65	-6.37	7.07E-04	suspension	1.79	4.34E-02

Bepridil	64706-54-3	1.00	25	73	5.44	-4.92	1.09E-03	suspension	2.86	7.91E-01
Bezafibrate	41859-67-0	1.00	186	73	2.50	-3.82	1.66E-03	suspension	1.07	1.94E-02
Bicalutamide	90357-06-5	0.90	192	73	4.14	-5.74	1.16E-04	suspension	2.16	1.69E-02
Bifemelane	90293-01-9	0.95	113	166	3.97	-3.49	1.86E-04	suspension	2.75	1.04E-01
Biperiden	514-65-8	1.00	101	73	4.27	-3.96	3.85E-05	suspension	3.55	1.37E-01
Boceprevir	394730-60-0	0.92	121.5	120	2.84	-4.52	4.62E-03	suspension	1.27	8.57E-02
Bosentan	147536-97-8	0.70	139	214	4.36	-6.00	4.53E-04	suspension	2.10	5.73E-02
Bromhexine	3572-43-8	0.70	237.7	73	4.80	-4.24	1.28E-04	suspension	1.67	5.90E-03
Bromocriptine	25614-03-3	0.28	216.5	73	8.60	-6.48	1.53E-04	suspension	1.80	9.61E-03
Bumetanide	28395-03-1	0.96	230.5	73	2.88	-4.82	2.75E-05	suspension	2.40	6.97E-03
Bupivacaine	38396-39-3	0.90	107.7	73	3.31	-3.07	7.80E-04	suspension	2.18	1.18E-01
Bupropion	34911-55-2	0.87	25	73	2.32	-2.74	1.88E-03	suspension	2.62	7.91E-01
Buspirone	36505-84-7	1.00	103.5	196	1.59	-3.68	1.56E-04	suspension	2.92	1.30E-01
Camazepam	36104-80-0	1.00	173.5	73	3.11	-3.68	5.38E-05	suspension	2.68	2.59E-02
Canagliflozin	842133-18-0	0.84	99	206	2.71	-5.23	6.75E-04	suspension	2.33	1.44E-01
Candoxatril	118785-03-8	0.38	108	73	3.28	-4.74	3.88E-04	suspension	2.48	1.17E-01
Capecitabine	154361-50-9	0.96	115.5	73	1.04	-3.17	1.13E-02	suspension	0.94	9.84E-02

Carbamazepine	298-46-4	1.00	191.5	73	1.90	-3.03	6.78E-03	suspension	0.40	1.71E-02
Carbamazepine10 11Epoxide	36507-30-9	0.90	192	119	0.16	-2.12	6.34E-03	suspension	0.43	1.69E-02
Carglumic Acid	1188-38-1	0.40	174	73	-0.74	-0.92	7.89E-02	suspension	-0.49	2.56E-02
Carprofen	53716-49-7	1.00	197.5	73	3.84	-5.27	2.19E-03	suspension	0.83	1.49E-02
Carvedilol	72956-09-3	0.80	114.5	73	4.07	-5.28	6.16E-05	suspension	3.21	1.01E-01
Cefaclor	53994-73-3	0.90	142	85	0.14	-3.23	4.08E-03	suspension	1.12	5.34E-02
Cefadroxil	50370-12-2	1.00	197	168	-0.25	-2.96	2.76E-03	suspension	0.74	1.51E-02
Cefazolin	25953-19-9	1.00	199	73	-0.70	-4.41	8.81E-03	suspension	0.21	1.44E-02
Cefixime	79350-37-1	0.60	300	169	-0.10	-3.82	1.76E-03	suspension	-0.10	1.41E-03
Cefmetazole	56796-20-4	0.10	151	114	-0.62	-4.40	1.27E-02	suspension	0.53	4.34E-02
Cefodizime	69739-16-8	0.00	213.5	152	0.52	-5.10	3.42E-03	suspension	0.48	1.03E-02
Cefoperazone	62893-19-0	0.10	170	73	-1.11	-4.24	1.86E-02	suspension	0.18	2.81E-02
Ceforanide	60925-61-3	0.00	150	73	-0.36	-4.11	3.85E-03	suspension	1.06	4.45E-02
Cefoxitin	35607-66-0	0.15	149.5	73	0.00	-3.85	2.81E-02	suspension	0.20	4.50E-02
Cefpodoxime proxetil	87239-81-4	0.50	99.5	217	2.95	-5.70	1.08E-03	suspension	2.12	1.42E-01
Cefprozil	92665-29-7	0.95	219	39	-0.60	-2.80	2.57E-03	suspension	0.55	9.08E-03
Ceftizoxime	68401-81-0	0.72	227	73	-0.65	-3.42	1.56E-02	suspension	-0.32	7.55E-03

Ceftriaxone	73384-59-5	0.01	156	215	-0.68	-4.72	7.22E-03	suspension	0.73	3.87E-02
Cefuroxime	55268-75-2	0.45	221.5	39	0.26	-3.68	2.36E-03	suspension	0.56	8.57E-03
Cefuroxime Axetil	64544-07-6	0.44	134.2	39	1.93	-4.96	1.96E-03	suspension	1.51	6.40E-02
Celecoxib	169590-42-5	0.97	158	73	2.59	-4.43	1.05E-03	suspension	1.55	3.70E-02
Celiprolol	56980-93-9	0.50	111	73	1.92	-3.13	1.05E-03	suspension	2.01	1.09E-01
Cephalexin	15686-71-2	0.96	197	125	0.35	-3.30	1.15E-02	suspension	0.12	1.51E-02
Cephalothin	153-61-7	0.00	160.2	73	0.09	-3.47	1.51E-02	suspension	0.37	3.52E-02
Cephradine	38821-53-3	0.95	182	155	0.48	-3.24	1.15E-02	suspension	0.27	2.13E-02
Cetirizine	83881-51-0	1.00	112.5	73	1.62	-2.17	2.59E-03	suspension	1.61	1.05E-01
Chenodeoxycholic Acid	474-25-9	1.00	119	73	4.76	-5.29	6.37E-04	suspension	2.15	9.08E-02
Chloramphenicol	56-75-7	0.89	151	73	1.10	-2.48	1.86E-02	suspension	0.37	4.34E-02
Chlorguanide	500-92-5	0.85	129	73	2.49	-3.05	7.87E-04	suspension	1.96	7.21E-02
Chlorhexidine	55-56-1	0.05	134	73	4.58	-5.70	7.12E-05	suspension	2.96	6.43E-02
Chlormezanone	80-77-3	1.00	117.2	73	0.48	-3.19	1.46E-03	suspension	1.81	9.46E-02
Chloroquine	54-05-7	1.00	87	73	4.41	-4.57	3.13E-03	suspension	1.78	1.90E-01
Chlorothiazide	58-94-6	0.60	350	39	-0.15	-3.25	6.76E-03	suspension	-1.18	4.45E-04
Chloroxine	773-76-2	0.89	179.5	73	3.07	-3.34	1.87E-02	suspension	0.08	2.25E-02

Chlorphenesin	104-29-0	1.00	78	73	1.71	-1.85	1.18E-02	suspension	1.29	2.33E-01
Chlorpromazine	50-53-3	0.98	58	126	5.18	-5.49	3.14E-03	suspension	2.07	3.70E-01
Chlorpropamide	94-20-2	0.95	128	73	2.30	-3.06	2.71E-03	suspension	1.43	7.38E-02
Chlorzoxazone	95-25-0	0.90	191.2	73	1.82	-2.15	1.18E-02	suspension	0.16	1.72E-02
Cibenzoline	53267-01-9	1.00	103.5	73	3.49	-4.15	7.62E-04	suspension	2.23	1.30E-01
Cilomilast	153259-65-5	1.00	157	73	2.11	-3.74	8.74E-05	suspension	2.64	3.78E-02
Cilostazol	73963-72-1	0.74	159.9	73	3.36	-5.04	5.41E-04	suspension	1.82	3.54E-02
Cimetidine	51481-61-9	0.87	142	73	-0.07	-2.54	9.51E-03	suspension	0.75	5.34E-02
Cinchonine	118-10-5	1.00	265	73	2.79	-3.20	7.13E-03	suspension	-0.36	3.15E-03
Cinolazepam	75696-02-5	0.95	191.5	73	2.24	-4.06	2.80E-05	suspension	2.79	1.71E-02
Cinoxacin	28657-80-9	0.95	261.5	73	0.49	-2.51	3.82E-03	suspension	-0.05	3.41E-03
Ciprofibrate	52214-84-3	0.99	115	73	2.93	-3.47	3.47E-04	suspension	2.46	9.95E-02
Ciprofloxacin	85721-33-1	0.69	256	73	1.63	-3.89	2.41E-03	suspension	0.21	3.87E-03
Cisapride	81098-60-4	0.98	109.8	95	2.83	-4.11	1.71E-04	suspension	2.82	1.12E-01
Citalopram	59729-33-8	1.00	93	91	3.48	-4.52	1.85E-04	suspension	2.95	1.65E-01
Clinafloxacin	105956-97-6	1.00	255.5	73	2.45	-5.04	1.09E-03	suspension	0.55	3.92E-03
Clobazam	22316-47-8	0.87	167	73	1.25	-3.64	2.66E-04	suspension	2.05	3.01E-02

Clofibrate	637-07-0	0.96	25	73	3.88	-3.49	8.23E-03	suspension	1.98	7.91E-01
Clomethiazole	533-45-9	0.95	25	73	1.71	-2.17	2.38E-03	suspension	2.52	7.91E-01
Clomiphene	911-45-5	0.90	113	136	5.85	-5.48	2.47E-04	suspension	2.63	1.04E-01
Clonazepam	1622-61-3	0.80	236.5	73	2.52	-4.12	2.53E-05	suspension	2.38	6.07E-03
Clopidogrel	113665-84-2	0.50	25	73	2.58	-3.52	2.33E-04	suspension	3.53	7.91E-01
Clozapine	5786-21-0	0.94	183.5	73	3.94	-4.85	2.75E-03	suspension	0.87	2.06E-02
Crizotinib	877399-52-5	0.47	194	111	3.55	-5.57	1.11E-03	suspension	1.16	1.61E-02
Cromolyn	16110-51-3	0.01	241.5	73	2.00	-5.41	1.70E-03	suspension	0.50	5.41E-03
Cyproheptadine	129-03-3	0.80	112.8	73	5.82	-4.43	1.04E-04	suspension	3.00	1.05E-01
Cyproterone acetate	427-51-0	0.98	238.7	73	4.22	-6.12	7.20E-04	suspension	0.90	5.77E-03
Cytarabine	147-94-4	0.20	212.5	73	-1.81	-6.33	6.66E-04	suspension	1.20	1.05E-02
Dantrolene	7261-97-4	0.80	279.5	73	1.07	-5.17	1.27E-03	suspension	0.25	2.25E-03
Dapsone	80-08-0	0.90	175.5	73	0.99	-3.18	1.21E-03	suspension	1.31	2.47E-02
Deferasirox	201530-41-8	0.81	264.5	73	5.15	-5.32	6.43E-03	suspension	-0.31	3.18E-03
Deferoxamine	70-51-9	0.02	139	121	-0.61	-2.47	1.07E-02	suspension	0.73	5.73E-02
Delavirdine	136817-59-9	0.85	227	73	3.53	-3.12	8.77E-04	suspension	0.94	7.55E-03
Dexamethasone	50-02-2	0.90	263	73	2.03	-4.05	2.29E-05	suspension	2.16	3.30E-03

Dexloxiglumide	119817-90-2	0.95	114	73	4.37	-4.01	4.33E-04	suspension	2.37	1.02E-01
Diacetylmorphine	561-27-3	1.00	173	73	1.58	-3.49	9.75E-04	suspension	1.43	2.62E-02
Diatrizoate	117-96-4	0.05	300	73	0.49	-2.89	4.73E-02	suspension	-1.53	1.41E-03
Diazepam	439-14-5	0.99	133	73	2.80	-3.74	1.41E-04	suspension	2.67	6.58E-02
Diazoxide	364-98-7	0.90	330.5	73	1.19	-2.80	2.08E-03	suspension	-0.48	6.97E-04
Diclofenac	15307-86-5	0.97	157	73	4.55	-4.89	7.60E-04	suspension	1.70	3.78E-02
Diethylstilbestrol	56-53-1	0.90	170.5	73	5.33	-4.60	2.24E-03	suspension	1.09	2.77E-02
Diflunisal	22494-42-4	0.90	212	73	3.65	-4.00	6.00E-03	suspension	0.25	1.07E-02
Dihydroergotamine	511-12-6	0.35	239	73	5.69	-5.14	3.43E-06	suspension	3.22	5.73E-03
Diloxanide	579-38-4	0.90	175	73	1.67	-1.70	6.41E-03	suspension	0.59	2.50E-02
Diltiazem	42399-41-7	0.91	106	230	4.73	-4.00	1.16E-03	suspension	2.02	1.22E-01
Diphenoxylate	915-30-0	0.90	222.5	193	4.51	-5.21	4.41E-05	suspension	2.28	8.37E-03
Disopyramide	9/5/3737	0.95	94.7	73	2.33	-3.24	4.71E-03	suspension	1.53	1.59E-01
Disulfiram	97-77-8	0.88	70	73	3.82	-5.10	1.69E-03	suspension	2.22	2.81E-01
Dolasetron	115956-12-2	0.85	231.5	172	2.57	-3.66	3.08E-04	suspension	1.34	6.81E-03
Domperidone	57808-66-9	0.95	242.5	73	4.05	-5.46	7.04E-05	suspension	1.88	5.28E-03
Dothiepin	113-53-1	0.95	56	73	4.27	-3.89	5.08E-04	suspension	2.88	3.87E-01

Doxazosin	74191-85-8	1.00	250	195	2.85	-5.24	3.55E-05	suspension	2.10	4.45E-03
Doxepin	1668-19-5	1.00	25	73	3.84	-3.77	1.07E-03	suspension	2.87	7.91E-01
Doxorubicin	23214-92-8	0.05	183	82	0.24	-4.52	2.68E-04	suspension	1.89	2.08E-02
Doxycycline	564-25-0	1.00	201	39	1.78	-4.89	4.50E-04	suspension	1.48	1.37E-02
Eltrombopag Olamine	496775-61-2	0.52	237.5	113	4.71	-5.32	3.39E-04	suspension	1.24	5.93E-03
Encainide	66778-36-7	0.95	131.2	130	3.75	-4.59	5.67E-04	suspension	2.08	6.85E-02
Enoxacin	74011-58-8	0.89	222	73	1.59	-2.72	3.75E-03	suspension	0.35	8.47E-03
Enoximone	77671-31-9	0.80	256.5	73	3.05	-3.80	1.51E-03	suspension	0.40	3.83E-03
Entacapone	130929-57-6	0.50	162.5	73	2.12	-2.13	5.24E-03	suspension	0.80	3.33E-02
Enzalutamide	915087-33-1	0.85	198	112	2.98	-5.82	3.45E-04	suspension	1.63	1.47E-02
Epristeride	119169-78-7	0.93	245.5	73	5.71	-5.96	1.25E-05	suspension	2.60	4.93E-03
Eprosartan	133040-01-4	0.15	260.5	73	2.96	-5.31	1.88E-03	suspension	0.27	3.49E-03
Ergotamine	113-15-5	1.00	213	73	7.37	-5.89	1.03E-05	suspension	3.00	1.04E-02
Erlotinib	183321-74-6	0.60	156.5	199	3.03	-4.80	7.63E-04	suspension	1.70	3.83E-02
Estramustine	2998-57-4	0.75	104.5	73	5.75	-6.74	2.18E-03	suspension	1.76	1.27E-01
Ethacrynic acid	58-54-8	0.90	121.5	73	2.84	-3.64	1.32E-03	suspension	1.81	8.57E-02
Ethynodiol diacetate	297-76-7	1.00	132	188	5.45	-5.92	2.61E-06	suspension	4.41	6.73E-02

Etodolac	41340-25-4	0.70	146.5	73	3.42	-3.36	4.18E-03	suspension	1.06	4.82E-02
Etoposide	33419-42-0	0.50	243.5	73	0.28	-4.21	2.75E-04	suspension	1.27	5.16E-03
Etoricoxib	202409-33-4	1.00	127.5	73	2.46	-3.82	3.34E-04	suspension	2.35	7.46E-02
Etravirine	269055-15-4	0.16	255	73	3.88	-7.27	9.19E-04	suspension	0.63	3.96E-03
Ezetimibe	163222-33-1	0.31	165	73	3.96	-5.37	2.44E-05	suspension	3.11	3.15E-02
Ezogabine	150812-12-7	0.84	141.5	73	0.96	-3.82	3.96E-03	suspension	1.14	5.41E-02
Famciclovir	104227-87-4	0.70	103	73	-0.12	-3.27	4.67E-03	suspension	1.45	1.31E-01
Febuxostat	144060-53-7	0.89	238.5	73	4.00	-4.96	3.79E-04	suspension	1.18	5.79E-03
Felbamate	25451-15-4	0.90	151.5	73	0.73	-1.80	1.51E-02	suspension	0.45	4.29E-02
Felodipine	72509-76-3	0.94	145	73	4.76	-5.28	5.20E-05	suspension	2.98	4.99E-02
Fenclofenac	34645-84-6	1.00	136	126	4.59	-5.00	2.02E-03	suspension	1.48	6.14E-02
Fenfluramine	458-24-2	0.95	25	73	3.55	-2.77	5.19E-04	suspension	3.18	7.91E-01
Fenofibrate	49562-28-9	0.90	80.5	73	5.80	-5.52	5.54E-04	suspension	2.60	2.20E-01
Fenoprofen	29679-58-1	0.85	25	73	3.72	-3.85	1.24E-02	suspension	1.81	7.91E-01
Fenspiride	6/5/5053	1.00	144	227	0.89	-2.54	1.84E-03	suspension	1.44	5.10E-02
Feprazone	30748-29-9	0.90	156.5	73	3.05	-3.85	2.34E-03	suspension	1.21	3.83E-02
Fidaxomicin	873857-62-6	0.08	163	73	9.14	-5.52	3.78E-04	suspension	1.94	3.30E-02

Finasteride	98319-26-7	1.00	257	73	3.83	-4.55	1.34E-05	suspension	2.45	3.78E-03
Flecainide	54143-55-4	0.81	93	156	3.19	-3.38	7.24E-04	suspension	2.36	1.65E-01
Fleroxacin	79660-72-3	1.00	272	102	1.84	-3.96	1.08E-03	suspension	0.39	2.68E-03
Fluconazole	86386-73-4	0.94	139	73	0.45	-3.01	2.61E-03	suspension	1.34	5.73E-02
Flunarizine	52468-60-7	0.80	97.5	225	5.59	-5.16	2.47E-05	suspension	3.78	1.49E-01
Fluocortolone	152-97-6	0.90	188.7	73	1.83	-3.77	2.66E-04	suspension	1.84	1.82E-02
Fluorescein	7/5/2321	0.99	315	73	2.68	-4.89	1.50E-03	suspension	-0.18	9.95E-04
Fluoxetine	54910-89-3	0.80	158	222	3.93	-3.74	2.58E-04	suspension	2.16	3.70E-02
Fluoxymesterone	76-43-7	0.44	270	73	2.27	-3.89	5.94E-05	suspension	1.67	2.81E-03
Flupirtine	56995-20-1	1.00	115.5	73	1.60	-3.49	1.97E-03	suspension	1.70	9.84E-02
Flurazepam	17617-23-1	1.00	79.5	73	4.84	-5.04	7.73E-05	suspension	3.46	2.25E-01
Flurbiprofen	5104-49-4	0.95	110.5	73	3.66	-3.89	1.23E-03	suspension	1.95	1.10E-01
Flutamide	13311-84-7	0.90	112	73	3.52	-3.89	2.72E-03	suspension	1.59	1.07E-01
Fluvoxamine	54739-18-3	0.90	25	174	3.71	-2.92	9.42E-04	suspension	2.92	7.91E-01
Folinic Acid	58-05-9	0.90	245	73	-1.43	-2.85	6.86E-04	suspension	0.86	4.99E-03
Fomepizole	7554-65-6	1.00	25	73	1.10	-1.37	2.19E-02	suspension	1.56	7.91E-01
Formoterol	73573-87-2	0.65	145.3	97	2.03	-3.42	4.65E-04	suspension	2.03	4.95E-02

Furosemide	54-31-9	0.61	206	73	2.30	-4.04	1.81E-03	suspension	0.83	1.22E-02
Fusidic acid	6/3/6990	1.00	192.5	73	5.76	-6.52	2.90E-03	suspension	0.76	1.67E-02
Gallopamil	16662-47-8	0.97	25	73	3.83	-4.77	4.64E-04	suspension	3.23	7.91E-01
Ganciclovir	82410-32-0	0.04	250	73	-1.61	-2.04	2.35E-03	suspension	0.28	4.45E-03
Gatifloxacin	112811-59-3	0.96	162	73	2.10	-4.29	1.33E-05	suspension	3.40	3.37E-02
Gemfibrozil	25812-30-0	1.00	62	73	4.30	-3.60	4.79E-03	suspension	1.85	3.37E-01
Gemifloxacin	175463-14-6	0.60	236	73	1.77	-3.85	8.22E-04	suspension	0.87	6.14E-03
Genaconazole	120924-80-3	1.00	147.5	201	1.48	-3.42	6.04E-04	suspension	1.89	4.71E-02
Glibornuride	26944-48-9	0.98	196.5	73	2.69	-3.66	1.36E-04	suspension	2.05	1.52E-02
Gliclazide	21187-98-4	0.97	181	73	1.61	-3.54	9.89E-04	suspension	1.34	2.18E-02
Glimepiride	93479-97-1	1.00	207	73	3.45	-5.26	1.63E-05	suspension	2.87	1.20E-02
Gliquidone	33342-05-1	0.95	181	73	3.91	-5.77	1.14E-04	suspension	2.28	2.18E-02
Glyburide	10238-21-8	0.98	169.5	73	3.08	-5.10	4.05E-05	suspension	2.85	2.84E-02
Glymidine	339-44-6	0.95	153	73	-0.07	-2.47	6.46E-03	suspension	0.81	4.15E-02
Griseofulvin	126-07-8	0.43	220	73	2.01	-3.96	2.13E-03	suspension	0.62	8.87E-03
Guanabenz	5051-62-7	0.78	228	73	2.66	-3.34	2.77E-04	suspension	1.43	7.38E-03
Haloperidol	52-86-8	1.00	148.7	73	3.76	-4.18	5.32E-05	suspension	2.93	4.58E-02

Hexobarbital	56-29-1	0.95	146	73	1.46	-2.30	2.12E-03	suspension	1.36	4.87E-02
Hydrocortisone	50-23-7	0.91	218.5	73	1.76	-3.59	6.62E-04	suspension	1.14	9.18E-03
Hydroxychloroquine	118-42-3	0.90	90	73	3.53	-3.80	1.79E-03	suspension	2.00	1.77E-01
Hydroxyprogesterone caproate	630-56-8	0.90	119	200	5.68	-6.02	5.83E-04	suspension	2.19	9.08E-02
Ibuprofen	15687-27-1	0.98	76	73	3.50	-3.04	1.16E-02	suspension	1.32	2.44E-01
Imatinib	152459-95-5	0.98	212	73	2.89	-4.77	1.62E-03	suspension	0.82	1.07E-02
Imipramine	50-49-7	0.98	174	202	4.36	-4.35	1.07E-03	suspension	1.38	2.56E-02
Indecainide	74517-78-5	1.00	94.5	73	3.87	-4.01	1.62E-03	suspension	1.99	1.60E-01
Indobufen	63610-08-2	1.00	183	73	3.33	-4.00	1.35E-03	suspension	1.19	2.08E-02
Indomethacin	53-86-1	1.00	158.5	73	4.25	-4.77	5.59E-04	suspension	1.82	3.66E-02
Indoprofen	31842-01-0	1.00	213.5	73	2.82	-3.66	7.11E-04	suspension	1.16	1.03E-02
Iohexol	66108-95-0	0.05	177	73	-2.92	-1.74	8.04E-03	suspension	0.47	2.39E-02
Iothalamic acid	2276-90-6	0.02	285	73	-0.06	-2.33	9.77E-03	suspension	-0.69	1.99E-03
Iotroxic acid	51022-74-3	0.05	300	150	4.32	-5.80	8.22E-03	suspension	-0.77	1.41E-03
Irbesartan	138402-11-6	1.00	180.5	73	5.25	-6.19	7.00E-04	suspension	1.50	2.20E-02
Isotretinoin	4759-48-2	0.90	174.5	73	6.26	-4.68	3.99E-04	suspension	1.80	2.53E-02
Isoxepac	55453-87-7	0.98	131.7	73	2.11	-4.28	7.46E-04	suspension	1.96	6.78E-02

Isoxicam	34552-84-6	1.00	268	73	0.90	-2.85	5.96E-04	suspension	0.69	2.94E-03
Isradipine	75695-93-1	0.92	169	73	3.73	-4.70	2.70E-05	suspension	3.03	2.87E-02
Itraconazole	84625-61-6	0.80	166.2	73	5.00	-6.85	8.50E-04	suspension	1.56	3.06E-02
Ivermectin	70288-86-7	0.60	155	73	6.92	-6.05	1.01E-05	suspension	3.59	3.96E-02
Ketanserin	74050-98-9	1.00	231	73	3.56	-4.74	2.02E-04	suspension	1.53	6.89E-03
Ketazolam	27223-35-4	1.00	182.7	73	0.51	-3.54	1.63E-04	suspension	2.11	2.09E-02
Ketoconazole	65277-42-1	0.75	146	73	4.04	-4.32	7.53E-04	suspension	1.81	4.87E-02
Ketoprofen	22071-15-4	0.95	94	73	2.91	-3.37	1.18E-03	suspension	2.14	1.61E-01
Ketorolac	74103-06-3	0.95	160.5	73	2.68	-3.48	5.88E-04	suspension	1.77	3.49E-02
Labetalol	36894-69-6	0.95	161	76	2.72	-3.06	7.31E-03	suspension	0.67	3.45E-02
Lacidipine	103890-78-4	0.98	174.5	73	5.99	-5.96	1.76E-05	suspension	3.16	2.53E-02
Lactulose	4618-18-2	0.01	169.5	73	-2.97	-0.51	1.17E-01	suspension	-0.61	2.84E-02
Lamotrigine	84057-84-1	0.98	217	73	1.24	-3.24	1.56E-03	suspension	0.78	9.50E-03
Lansoprazole	103577-45-3	0.85	180	73	2.58	-4.77	8.12E-05	suspension	2.44	2.23E-02
Leflunomide	75706-12-6	0.80	165.5	140	2.29	-3.77	7.39E-05	suspension	2.62	3.11E-02
Lercanidipine	100427-26-7	0.44	54	94	7.56	-7.25	4.90E-05	suspension	3.92	4.05E-01
Levofloxacin	100986-85-4	1.00	226	73	1.86	-3.72	2.08E-03	suspension	0.57	7.73E-03

Levomepromazine	60-99-1	0.53	117	73	4.94	-5.19	6.08E-04	suspension	2.19	9.50E-02
Linezolid	165800-03-3	1.00	182	73	0.45	-2.96	3.56E-03	suspension	0.78	2.13E-02
Lomefloxacin	98079-51-7	0.99	239.7	73	2.46	-4.17	1.14E-03	suspension	0.69	5.64E-03
Lomustine	13010-47-4	1.00	90	73	2.72	-2.66	9.01E-04	suspension	2.29	1.77E-01
Loperamide Hydrochloride	53179-11-6	0.76	103.5	236	4.15	-3.96	3.35E-05	suspension	3.59	1.30E-01
Lopinavir	192725-17-0	0.81	125.5	73	5.42	-6.24	1.27E-03	suspension	1.79	7.82E-02
Loratadine	79794-75-5	0.90	135	73	3.90	-4.70	2.62E-05	suspension	3.38	6.28E-02
Lorcainide	59729-31-6	0.70	104.9	77	3.62	-3.85	1.08E-03	suspension	2.07	1.26E-01
Losartan	114798-26-4	0.80	184	73	3.46	-5.25	2.37E-04	suspension	1.93	2.03E-02
Lovastatin	75330-75-5	0.31	174.5	73	4.31	-4.70	1.97E-04	suspension	2.11	2.53E-02
Loxiglumide	107097-80-3	1.00	114	73	4.37	-4.01	1.73E-03	suspension	1.77	1.02E-01
Loxoprofen	68767-14-6	0.58	25	73	1.69	-2.82	7.31E-04	suspension	3.03	7.91E-01
Lymecycline	992-21-2	1.00	200	126	0.75	-3.82	6.77E-04	suspension	1.32	1.41E-02
Lynestrenol	52-76-6	1.00	159	73	5.59	-5.64	1.76E-05	suspension	3.31	3.61E-02
Maprotiline	10262-69-8	0.98	93	73	4.36	-4.30	8.11E-04	suspension	2.31	1.65E-01
Maraviroc	376348-65-1	0.75	197.5	73	5.30	-6.33	1.17E-03	suspension	1.11	1.49E-02
Mebendazole	31431-39-7	1.00	288.5	73	2.83	-4.85	6.77E-04	suspension	0.43	1.83E-03

Mebeverine	6/7/3625	0.90	130	212	5.77	-4.96	9.43E-04	suspension	1.87	7.05E-02
Meclofenamic acid	644-62-2	1.00	258	73	5.44	-5.37	1.35E-03	suspension	0.44	3.70E-03
Mefenamic acid	61-68-7	0.90	230.5	73	4.83	-4.29	5.17E-03	suspension	0.13	6.97E-03
Mefloquine	53230-10-7	0.78	175	73	2.00	-3.23	3.30E-03	suspension	0.88	2.50E-02
Megestrol acetate	595-33-5	1.00	215	73	3.75	-4.77	2.08E-03	suspension	0.68	9.95E-03
Meloxicam	71125-38-7	0.90	254	73	2.66	-4.11	4.27E-05	suspension	1.98	4.05E-03
Meptazinol	54340-58-8	1.00	130.2	73	3.40	-2.09	6.86E-03	suspension	1.01	7.01E-02
Meropenem	96036-03-2	0.00	235	154	-1.23	-1.89	1.56E-02	suspension	-0.40	6.28E-03
Mesalamine	89-57-6	0.80	280	73	0.74	-1.12	2.61E-02	suspension	-1.07	2.23E-03
Methadone	76-99-3	0.80	78	73	3.93	-3.82	9.69E-05	suspension	3.38	2.33E-01
Methocarbamol	532-03-6	1.00	93	73	0.40	-1.19	2.49E-02	suspension	0.82	1.65E-01
Methotrexate	59-05-2	0.70	185.5	126	-0.45	-4.21	6.60E-05	suspension	2.47	1.96E-02
Methsuximide	77-41-8	1.00	52.5	73	0.42	-2.03	5.90E-03	suspension	1.85	4.20E-01
Methylphenobarbital	115-38-8	0.50	176	73	1.23	-2.40	2.44E-03	suspension	1.00	2.44E-02
Methylprednisolone	83-43-2	0.82	232.5	73	2.17	-3.89	6.68E-04	suspension	1.00	6.65E-03
Metolazone	17560-51-9	0.64	253	73	3.16	-4.92	5.47E-05	suspension	1.88	4.15E-03
Metyrapone	54-36-4	0.80	50.5	73	1.14	-1.89	1.99E-02	suspension	1.34	4.39E-01

Mezlocillin	51481-65-3	0.00	170	191	0.33	-4.42	2.97E-02	suspension	-0.02	2.81E-02
Miconazole	22916-47-8	0.99	86	234	4.97	-5.68	8.65E-03	suspension	1.35	1.94E-01
Midazolam	59467-70-8	1.00	159	73	3.80	-4.96	1.53E-05	suspension	3.37	3.61E-02
Mifepristone	84371-65-3	0.90	150	73	6.19	-7.89	1.40E-03	suspension	1.50	4.45E-02
Minocycline	10118-90-8	1.00	164	99	2.12	-5.48	4.37E-04	suspension	1.87	3.22E-02
Minoxidil	51384-51-1	0.96	248	73	1.62	-3.24	4.78E-04	suspension	0.99	4.66E-03
Mitotane	53-19-0	0.40	77	73	5.41	-6.49	1.87E-02	suspension	1.10	2.39E-01
Mitoxantrone	65271-80-9	0.05	161	73	1.55	-4.46	4.50E-05	suspension	2.88	3.45E-02
Montelukast	158966-92-8	0.80	147.5	226	5.81	-7.44	1.71E-05	suspension	3.44	4.71E-02
Moricizine	31883-05-3	0.88	156.5	73	2.36	-4.51	2.11E-03	suspension	1.26	3.83E-02
Moxalactam	64952-97-2	0.00	119.5	73	-2.56	-2.39	7.69E-03	suspension	1.07	8.97E-02
Moxifloxacin	151096-09-2	0.90	205.5	73	2.83	-5.17	9.96E-04	suspension	1.09	1.24E-02
Moxisylyte	54-32-0	0.70	144.5	39	3.17	-3.06	1.14E-03	suspension	1.64	5.05E-02
Mycophenolic Acid	24280-93-1	0.83	141	73	3.84	-3.77	2.25E-02	suspension	0.39	5.47E-02
Nabumetone	42924-53-8	0.80	80	73	3.14	-3.57	8.76E-03	suspension	1.41	2.23E-01
Nafronyl	31329-57-4	1.00	190	95	3.91	-4.66	1.56E-03	suspension	1.05	1.77E-02
Nalidixic acid	389-08-2	0.90	229.5	73	0.03	-2.72	1.72E-02	suspension	-0.38	7.13E-03

Naltrexone	16590-41-3	0.95	169	73	2.05	-3.00	4.39E-04	suspension	1.82	2.87E-02
Naproxen	22204-53-1	0.99	153	73	2.88	-3.33	6.51E-03	suspension	0.80	4.15E-02
Nateglinide	105816-04-4	0.83	129.5	73	2.35	-3.35	1.13E-03	suspension	1.80	7.13E-02
Nedocromil	69049-73-6	0.03	299	73	1.30	-5.55	3.76E-05	suspension	1.58	1.44E-03
Nefazodone	83366-66-9	1.00	83.5	73	4.09	-5.29	1.28E-03	suspension	2.21	2.06E-01
Nelfinavir	159989-64-7	0.78	185.5	213	7.28	-5.82	4.40E-03	suspension	0.65	1.96E-02
Nevirapine	129618-40-2	1.00	248	73	2.64	-3.14	1.50E-03	suspension	0.49	4.66E-03
Nicardipine	55985-32-5	0.95	77	208	4.89	-5.74	2.50E-04	suspension	2.98	2.39E-01
Nifedipine	21829-25-4	0.90	173	73	3.58	-4.47	5.20E-04	suspension	1.70	2.62E-02
Nilutamide	63612-50-0	1.00	149	73	1.94	-3.60	9.46E-04	suspension	1.68	4.55E-02
Nilvadipine	75530-68-6	1.00	149	73	3.38	-5.14	4.15E-05	suspension	3.04	4.55E-02
Nimodipine	66085-59-4	1.00	125	73	4.05	-4.96	8.60E-04	suspension	1.96	7.91E-02
Nisoldipine	63675-72-9	0.90	151.5	73	4.96	-5.34	1.03E-04	suspension	2.62	4.29E-02
Nitisinone	104206-65-7	0.90	91	73	0.99	-3.52	3.64E-04	suspension	2.68	1.73E-01
Nitrendipine	39562-70-4	0.88	158	73	3.81	-4.64	5.54E-05	suspension	2.82	3.70E-02
Nitrofurantoin	67-20-9	0.95	271	73	-0.47	-3.52	1.68E-03	suspension	0.21	2.74E-03
Nitroxoline	4008-48-4	1.00	180.5	73	2.00	-2.55	3.16E-03	suspension	0.84	2.20E-02

Norfloxacin	70458-96-7	0.75	220.5	73	1.74	-3.35	2.51E-03	suspension	0.54	8.77E-03
Norgestimate	35189-28-7	1.00	216	73	5.13	-5.64	6.77E-07	suspension	4.16	9.73E-03
Nortriptyline	72-69-5	1.00	54	178	3.97	-3.60	3.80E-04	suspension	3.03	4.05E-01
Ofloxacin	82419-36-1	1.00	253.5	73	1.86	-3.72	2.21E-03	suspension	0.27	4.10E-03
Olanzapine	132539-06-1	1.00	195	73	3.08	-4.28	4.80E-05	suspension	2.52	1.58E-02
Olopatadine	113806-05-6	0.70	188.7	73	2.96	-3.64	5.92E-05	suspension	2.49	1.82E-02
Olsalazine	15722-48-2	0.08	300	148	3.57	-4.07	3.32E-03	suspension	-0.37	1.41E-03
Omeprazole	73590-58-6	0.80	156	73	2.36	-4.06	3.47E-04	suspension	2.05	3.87E-02
Ondansetron	99614-02-5	1.00	231.5	73	1.56	-3.89	8.18E-05	suspension	1.92	6.81E-03
Orlistat	96829-58-2	0.17	43	73	7.00	-7.32	7.26E-04	suspension	2.86	5.22E-01
Orphenadrine	83-98-7	1.00	25	73	3.33	-2.96	1.49E-03	suspension	2.73	7.91E-01
Oxamniquine	21738-42-1	0.80	148	73	2.02	-1.92	1.29E-02	suspension	0.56	4.66E-02
Oxandrolone	53-39-4	0.97	236.5	73	3.39	-3.62	6.52E-05	suspension	1.97	6.07E-03
Oxaprozin	21256-18-8	0.98	161	73	3.15	-3.66	6.14E-03	suspension	0.75	3.45E-02
Oxatomide	60607-34-3	1.00	153.6	73	4.34	-5.37	2.81E-04	suspension	2.16	4.09E-02
Oxazepam	604-75-1	0.97	205.5	73	2.22	-2.85	4.19E-04	suspension	1.47	1.24E-02
Oxcarbazepine	28721-07-5	1.00	215.5	73	1.66	-3.11	4.76E-03	suspension	0.32	9.84E-03

Oxybutynin	5633-20-5	1.00	56	96	5.05	-4.59	5.59E-05	suspension	3.84	3.87E-01
Oxyphenbutazone	129-20-4	1.00	124.5	73	2.74	-3.66	3.08E-04	suspension	2.41	8.00E-02
Oxytetracycline	79-57-2	0.58	185	149	0.48	-4.33	4.34E-03	suspension	0.66	1.99E-02
Pafenolol	75949-61-0	0.29	132	78	1.66	-4.96	2.96E-04	suspension	2.36	6.73E-02
Pantoprazole	102625-70-7	0.77	139.5	73	1.57	-4.17	1.04E-04	suspension	2.73	5.66E-02
Papaverine	58-74-2	0.90	147	73	2.93	-4.00	1.77E-03	suspension	1.43	4.76E-02
Pefloxacin	70458-92-3	0.95	271	73	1.92	-3.39	2.40E-03	suspension	0.06	2.74E-03
Penbutolol	38363-40-5	1.00	70	73	4.02	-3.15	2.74E-04	suspension	3.01	2.81E-01
Penicillin G	61-33-6	0.30	217	237	1.92	-2.89	3.58E-02	suspension	-0.58	9.50E-03
Penicillin V	87-08-1	0.59	124	73	1.94	-2.85	4.28E-03	suspension	1.28	8.09E-02
Pentamidine	100-33-4	0.00	186	73	2.85	-4.05	7.05E-04	suspension	1.44	1.94E-02
Pentazocine	359-83-1	0.95	147	73	4.15	-3.22	5.26E-04	suspension	1.96	4.76E-02
Pentobarbital	76-74-4	1.00	129.5	73	2.18	-2.70	8.83E-04	suspension	1.91	7.13E-02
Perhexiline	6621-47-2	0.80	244.2	95	6.47	-4.49	1.08E-03	suspension	0.67	5.08E-03
Perphenazine	58-39-9	1.00	97	73	3.94	-4.17	5.94E-05	suspension	3.40	1.51E-01
Phenacemide	63-98-9	1.00	214	73	0.87	-2.04	1.68E-02	suspension	-0.22	1.02E-02
Phenazopyridine	94-78-0	0.90	136.5	73	2.21	-3.35	1.88E-03	suspension	1.51	6.07E-02

Phenindione	83-12-5	1.00	150	73	3.13	-4.60	8.99E-04	suspension	1.69	4.45E-02
Phenprocoumon	435-97-2	0.95	179.5	73	4.64	-4.72	8.56E-05	suspension	2.42	2.25E-02
Phensuximide	86-34-0	1.00	72	73	0.04	-1.92	1.59E-02	suspension	1.23	2.68E-01
Phenylbutazone	50-33-9	0.98	105	73	3.38	-4.04	1.95E-03	suspension	1.81	1.25E-01
Phenylethylmalonamide	7206-76-0	0.91	124	135	0.35	-2.14	1.94E-03	suspension	1.62	8.09E-02
Phenytoin	57-41-0	0.90	295.5	73	1.42	-3.11	1.19E-03	suspension	0.12	1.56E-03
Phthalylsulfathiazole	85-73-4	0.05	274.5	73	0.80	-4.41	2.97E-02	suspension	-1.07	2.53E-03
Pimozide	2062-78-4	0.70	216	73	5.76	-5.96	2.17E-05	suspension	2.65	9.73E-03
Pioglitazone	111025-46-8	0.83	183.5	73	3.50	-4.52	8.42E-05	suspension	2.39	2.06E-02
Pipemidic Acid	51940-44-4	0.93	254	73	-0.19	-2.06	2.63E-03	suspension	0.19	4.05E-03
Piperacillin	61477-96-1	0.00	168	170	1.00	-4.41	4.64E-02	suspension	-0.20	2.94E-02
Pirazolac	71002-09-0	0.94	148.5	73	3.84	-4.70	1.81E-03	suspension	1.40	4.60E-02
Pirmenol	68252-19-7	0.95	70.5	73	3.57	-2.89	4.43E-04	suspension	2.80	2.77E-01
Posaconazole	171228-49-2	0.96	171	73	4.67	-6.36	8.56E-04	suspension	1.51	2.74E-02
Pranlukast	103177-37-3	0.20	232	104	4.05	-5.85	1.87E-03	suspension	0.56	6.73E-03
Pravastatin	81093-37-0	0.34	326	165	2.21	-3.85	9.43E-05	suspension	0.91	7.73E-04
Praziquantel	55268-74-1	0.96	137	73	2.66	-3.37	1.44E-02	suspension	0.62	6.00E-02

Prazosin	19216-56-9	0.86	279	73	2.14	-4.42	5.22E-05	suspension	1.64	2.28E-03
Prednisolone	50-24-8	0.99	240.5	73	1.64	-3.55	5.54E-04	suspension	1.00	5.53E-03
Prednisone	53-03-2	0.95	234	73	1.57	-3.55	1.67E-04	suspension	1.58	6.43E-03
Primidone	125-33-7	0.75	281.5	73	0.83	-2.15	2.29E-03	suspension	-0.03	2.15E-03
Probenecid	57-66-9	1.00	195	73	2.51	-3.06	3.51E-03	suspension	0.65	1.58E-02
Probucol	23288-49-5	0.07	125.2	73	9.00	-8.10	1.93E-03	suspension	1.61	7.87E-02
Procainamide	51-06-9	0.85	73.5	220	1.32	-1.60	1.27E-02	suspension	1.31	2.59E-01
Progesterone	57-83-0	0.96	121	73	3.83	-4.52	1.27E-03	suspension	1.83	8.67E-02
Promazine	58-40-2	1.00	25	73	4.69	-4.82	3.52E-03	suspension	2.35	7.91E-01
Promethazine	60-87-7	0.95	60	73	4.89	-4.89	3.52E-04	suspension	3.00	3.53E-01
Propafenone	54063-53-5	0.95	65	122	3.35	-3.46	2.64E-03	suspension	2.08	3.15E-01
Propofol	2078-54-8	1.00	25	73	3.66	-2.80	8.41E-04	suspension	2.97	7.91E-01
Propoxyphene	469-62-5	0.95	75.5	73	4.10	-4.07	1.15E-03	suspension	2.33	2.47E-01
Propranolol	525-66-6	0.95	96	73	2.90	-2.74	2.48E-03	suspension	1.79	1.54E-01
Propylthiouracil	51-52-5	0.76	220	73	1.15	-2.62	5.29E-03	suspension	0.22	8.87E-03
Protriptyline	438-60-8	0.95	166	124	4.36	-3.70	2.28E-04	suspension	2.13	3.08E-02
Pyrimethamine	58-14-0	1.00	233.5	73	2.75	-3.77	3.02E-04	suspension	1.33	6.50E-03

Quetiapine	111974-69-7	0.73	67.5	161	2.60	-4.18	2.08E-03	suspension	2.15	2.97E-01
Quinaprilat	82768-85-2	0.61	167	73	5.18	-4.20	9.75E-05	suspension	2.49	3.01E-02
Quinidine	56-54-2	0.80	174.5	73	2.82	-3.35	1.85E-03	suspension	1.14	2.53E-02
Quinine	130-95-0	0.85	177	73	2.82	-3.35	5.99E-03	suspension	0.60	2.39E-02
Rabeprazole	117976-89-3	0.90	99.5	73	2.10	-3.89	3.34E-04	suspension	2.63	1.42E-01
Raloxifene	84449-90-1	0.60	145	73	4.57	-5.09	1.27E-03	suspension	1.60	4.99E-02
Ramipril	87333-19-5	0.60	109	73	4.37	-4.22	4.80E-05	suspension	3.38	1.14E-01
Repaglinide	135062-02-1	1.00	127	73	4.88	-4.72	3.54E-05	suspension	3.33	7.55E-02
Retinol	68-26-8	0.80	63	73	6.08	-6.57	1.92E-04	suspension	3.23	3.30E-01
Ribavirin	36791-04-5	0.85	167	73	-1.85	-1.66	4.91E-02	suspension	-0.21	3.01E-02
Rifabutin	72559-06-9	0.53	152	88	4.49	-4.48	7.08E-04	suspension	1.78	4.25E-02
Rifampin	13292-46-1	0.80	185.5	73	2.05	-2.96	1.46E-03	suspension	1.13	1.96E-02
Rilpivirine	500287-72-9	0.75	242	73	4.53	-6.59	6.82E-05	suspension	1.89	5.34E-03
Riluzole	1744-22-5	0.90	119	73	2.92	-3.85	4.27E-04	suspension	2.33	9.08E-02
Risperidone	106266-06-2	0.97	170	73	2.68	-4.55	3.90E-05	suspension	2.86	2.81E-02
Ritonavir	155213-67-5	0.70	122	90	2.33	-4.57	1.66E-03	suspension	1.71	8.47E-02
Rivaroxaban	366789-02-8	0.66	232.5	73	1.71	-4.74	6.88E-05	suspension	1.99	6.65E-03

Rosiglitazone	122320-73-4	1.00	154	73	3.02	-4.38	2.23E-05	suspension	3.26	4.05E-02
Rufinamide	106308-44-5	0.85	238.5	73	1.00	-2.77	1.34E-02	suspension	-0.37	5.79E-03
Ruxolitinib	941678-49-5	0.95	88	145	2.07	-4.74	1.63E-04	suspension	3.06	1.85E-01
Saccharin	81-07-2	0.91	229.2	73	0.91	-2.08	1.09E-02	suspension	-0.18	7.18E-03
Salsalate	552-94-3	1.00	148.5	73	2.76	-3.89	1.55E-02	suspension	0.47	4.60E-02
Sertraline	79617-96-2	0.86	66.5	146	5.08	-4.77	6.52E-04	suspension	2.67	3.04E-01
Sibutramine	106650-56-0	0.77	53	176	5.47	-4.43	5.36E-05	suspension	3.89	4.15E-01
Sildenafil	139755-83-2	0.92	188	73	2.47	-4.96	2.11E-04	suspension	1.94	1.85E-02
Sitafloxacin	127254-12-0	0.95	225	186	2.62	-5.25	6.10E-04	suspension	1.11	7.91E-03
Sitagliptin	486460-32-6	0.95	25	73	2.06	-4.82	2.46E-04	suspension	3.51	7.91E-01
Solifenacin	242478-37-1	1.00	25	73	4.16	-4.55	2.76E-05	suspension	4.46	7.91E-01
Sparfloxacin	110871-86-8	0.90	267.5	73	2.60	-5.12	1.02E-03	suspension	0.46	2.97E-03
Spironolactone	52-01-7	0.73	134.5	73	3.15	-5.28	9.60E-04	suspension	1.82	6.35E-02
Succinylsulfathiazole	116-43-8	0.05	187	115	0.19	-2.59	2.70E-02	suspension	-0.15	1.90E-02
Sudoxicam	34042-85-8	1.00	248	197	2.36	-3.96	1.48E-04	suspension	1.50	4.66E-03
Sulbactam	68373-14-8	0.05	154.7	73	0.39	-2.06	1.72E-02	suspension	0.37	3.99E-02
Sulfadiazine	68-35-9	0.93	254	73	-0.07	-2.49	1.60E-02	suspension	-0.60	4.05E-03

Sulfamerazine	127-79-7	0.81	236	73	0.11	-2.72	1.51E-02	suspension	-0.39	6.14E-03
Sulfamethazine	57-68-1	0.95	198.5	39	0.30	-2.96	1.08E-02	suspension	0.13	1.46E-02
Sulfamethizole	144-82-1	0.85	208	73	0.52	-2.70	1.48E-02	suspension	-0.10	1.17E-02
Sulfamethoxazole	723-46-6	1.00	167	73	0.66	-2.82	6.32E-03	suspension	0.68	3.01E-02
Sulfapyridine	144-83-2	0.70	190.5	73	0.47	-2.51	2.41E-02	suspension	-0.14	1.75E-02
Sulfinpyrazone	57-96-5	1.00	136.5	73	1.89	-4.28	1.97E-03	suspension	1.49	6.07E-02
Sulfisomidine	515-64-0	0.90	243	73	0.58	-3.00	1.44E-02	suspension	-0.44	5.22E-03
Sulfisoxazole	127-69-5	0.95	194	73	1.01	-3.12	1.50E-02	suspension	0.03	1.61E-02
Sulindac	38194-50-2	0.90	183.5	73	2.55	-4.48	1.12E-03	suspension	1.26	2.06E-02
Sulphasalazine	599-79-1	0.13	242.5	73	3.05	-5.24	2.00E-02	suspension	-0.58	5.28E-03
Sulpiride	15676-16-1	0.40	179	73	0.78	-2.00	9.37E-03	suspension	0.39	2.28E-02
Sultopride	53583-79-2	0.89	181.5	39	1.39	-2.40	3.39E-03	suspension	0.80	2.15E-02
Suprofen	40828-46-4	0.92	124.3	73	2.18	-3.34	3.07E-03	suspension	1.42	8.03E-02
Tacrine	321-64-2	0.95	183.5	73	2.56	-3.26	8.07E-04	suspension	1.41	2.06E-02
Tacrolimus	104987-11-3	0.15	128	232	4.79	-4.64	2.01E-05	suspension	3.56	7.38E-02
Talinolol	38649-73-9	0.65	143	73	2.98	-3.80	8.25E-04	suspension	1.80	5.22E-02
Tamoxifen	10540-29-1	1.00	97	73	5.13	-4.80	1.08E-04	suspension	3.15	1.51E-01

Tapentadol	175591-23-8	0.99	79.6	108	3.02	-2.36	2.71E-03	suspension	1.92	2.25E-01
Tegaserod	145158-71-0	0.50	155	73	3.22	-3.96	3.98E-05	suspension	3.00	3.96E-02
Teicoplanin A2 1	91032-34-7	0.00	255	73	1.51	-10.62	2.13E-04	suspension	1.27	3.96E-03
Telithromycin	191114-48-4	0.90	187.5	73	5.22	-3.21	9.85E-04	suspension	1.28	1.87E-02
Telmisartan	144701-48-4	0.90	262	73	6.48	-6.89	1.55E-04	suspension	1.34	3.37E-03
Temocapril	111902-57-9	0.60	168	73	6.57	-5.46	8.39E-06	suspension	3.54	2.94E-02
Tenidap	120210-48-2	0.89	230	73	1.59	-3.23	3.74E-04	suspension	1.27	7.05E-03
Terbinafine	91161-71-6	0.80	193.5	89	5.58	-5.74	5.56E-03	suspension	0.47	1.63E-02
Terfenadine	50679-08-8	1.00	147.5	73	5.62	-5.49	2.54E-04	suspension	2.27	4.71E-02
Terodiline	15793-40-5	1.00	25	73	4.68	-4.12	1.78E-04	suspension	3.65	7.91E-01
Testosterone	58-22-0	1.00	155	73	3.18	-4.15	3.47E-04	suspension	2.06	3.96E-02
Tetrabenazine	58-46-8	1.00	127.5	73	2.93	-3.23	1.58E-04	suspension	2.68	7.46E-02
Tetracycline	60-54-8	0.80	172.5	73	0.62	-4.31	4.50E-03	suspension	0.77	2.65E-02
Tetrahydrocannabinol	8/3/1972	0.93	65.5	137	6.84	-5.60	6.36E-05	suspension	3.69	3.11E-01
Thiabendazole	148-79-8	0.90	304.5	73	2.47	-3.52	1.49E-02	suspension	-1.07	1.27E-03
Thiacetazone	104-06-3	0.20	227.5	73	1.49	-3.39	6.35E-04	suspension	1.07	7.46E-03
Thioridazine	50-52-2	0.60	73	73	5.90	-6.15	2.15E-03	suspension	2.08	2.62E-01

Tiacrilast	78299-53-3	0.99	273	198	1.44	-2.85	2.86E-03	suspension	-0.04	2.62E-03
Tiagabine	115103-54-3	0.90	83	228	4.03	-4.38	1.71E-04	suspension	3.09	2.08E-01
Tianeptine	72797-41-2	0.99	144	209	4.13	-5.19	8.58E-05	suspension	2.77	5.10E-02
Ticagrelor	274693-27-5	0.73	139	160	2.02	-5.02	3.44E-04	suspension	2.22	5.73E-02
Ticarcillin	34787-01-4	0.05	187.5	79	1.24	-2.92	4.68E-02	suspension	-0.40	1.87E-02
Ticlopidine	55142-85-3	0.80	209.5	81	3.23	-3.52	9.48E-04	suspension	1.08	1.13E-02
Tiludronic acid	89987-06-4	0.06	175.5	233	2.00	-3.01	1.26E-03	suspension	1.29	2.47E-02
Tinidazole	19387-91-8	1.00	127.5	73	-0.29	-1.89	8.08E-03	suspension	0.97	7.46E-02
Tizanidine	51322-75-9	1.00	222	73	2.39	-3.92	1.42E-04	suspension	1.78	8.47E-03
Tolbutamide	64-77-7	0.90	129	73	2.36	-2.92	7.39E-03	suspension	0.99	7.21E-02
Tolmetin	26171-23-3	0.99	156	73	2.68	-3.24	7.00E-03	suspension	0.74	3.87E-02
Tolrestat	82964-04-3	0.66	164.5	73	3.59	-4.96	5.60E-04	suspension	1.76	3.18E-02
Tolterodine	124937-51-5	0.77	78.5	218	5.23	-4.44	1.47E-03	suspension	2.19	2.31E-01
Topiramate	97240-79-4	0.86	125.5	73	2.16	-3.55	1.18E-03	suspension	1.82	7.82E-02
Toremifene	89778-26-7	1.00	109	73	4.77	-4.92	4.92E-04	suspension	2.37	1.14E-01
Torsemide	56211-40-6	0.96	163.5	73	1.96	-3.34	5.73E-04	suspension	1.75	3.26E-02
Trandolapril	87679-37-6	0.50	125	73	4.90	-4.41	7.43E-05	suspension	3.03	7.91E-02

Trapidil	15421-84-8	0.96	98.7	73	2.31	-2.89	2.92E-03	suspension	1.70	1.45E-01
Trazodone	19794-93-5	1.00	86.5	73	2.76	-4.40	1.61E-03	suspension	2.08	1.92E-01
Treosulfan	299-75-2	0.97	77	194	-0.77	-1.89	3.88E-03	suspension	1.79	2.39E-01
Triamcinolone	124-94-7	1.00	270	73	0.53	-3.22	2.54E-04	suspension	1.04	2.81E-03
Triamcinolone acetonide	76-25-5	0.90	293	73	2.43	-4.00	2.30E-04	suspension	0.86	1.65E-03
Trifluoperazine	117-89-5	1.00	232.5	239	4.62	-4.74	9.82E-05	suspension	1.83	6.65E-03
Trimeprazine	84-96-8	0.80	68	73	5.04	-5.11	3.36E-04	suspension	2.94	2.94E-01
Trimethoprim	738-70-5	0.97	201	73	0.59	-2.77	1.10E-03	suspension	1.10	1.37E-02
Trimipramine	739-71-9	0.80	45	73	4.71	-4.64	6.79E-04	suspension	2.87	4.99E-01
Ursodiol	128-13-2	1.00	203	73	4.76	-5.29	1.53E-03	suspension	0.93	1.31E-02
Valdecoxib	181695-72-7	0.83	156	73	3.57	-4.33	1.27E-04	suspension	2.48	3.87E-02
Valproic acid	99-66-1	0.98	25	73	2.58	-1.80	1.73E-02	suspension	1.66	7.91E-01
Valsartan	137862-53-4	0.55	116.5	73	4.02	-5.00	7.34E-04	suspension	2.12	9.61E-02
Vardenafil	224785-90-4	0.90	184	110	3.64	-5.59	4.09E-05	suspension	2.70	2.03E-02
Verapamil	52-53-9	0.95	25	73	4.02	-4.80	1.06E-03	suspension	2.87	7.91E-01
Vidarabine	5536-17-4	0.00	257.2	73	-0.76	-1.60	6.74E-03	suspension	-0.25	3.77E-03
Vilazodone	163521-12-8	0.98	235	175	3.98	-6.33	9.06E-05	suspension	1.84	6.28E-03

Vinblastine	865-21-4	0.05	213.5	73	5.92	-4.37	3.70E-05	suspension	2.45	1.03E-02
Viomycin	32988-50-4	0.85	258	187	-4.33	-2.15	5.84E-03	suspension	-0.20	3.70E-03
Vismodegib	879085-55-9	0.69	187	116	2.03	-5.51	3.56E-04	suspension	1.73	1.90E-02
Vitamin E	59-02-9	0.65	25	216	10.96	-7.92	6.97E-04	suspension	3.06	7.91E-01
Voriconazole	137234-62-9	0.96	127	73	1.21	-3.92	1.15E-03	suspension	1.82	7.55E-02
Warfarin	81-81-2	0.97	161	73	3.13	-4.20	3.25E-05	suspension	3.03	3.45E-02
Xipamide	14293-44-8	0.80	256	73	2.19	-4.74	1.13E-04	suspension	1.54	3.87E-03
Zaleplon	151319-34-5	1.00	186.5	73	1.40	-3.89	9.83E-05	suspension	2.29	1.92E-02
Zileuton	111406-87-2	1.00	157.5	73	2.70	-3.62	1.02E-02	suspension	0.57	3.74E-02
Ziprasidone	146939-27-7	0.60	219	93	2.97	-4.82	3.88E-04	suspension	1.37	9.08E-03
Zomepirac	33369-31-2	1.00	178.5	73	3.36	-3.85	2.06E-03	suspension	1.05	2.31E-02
Zonisamide	68291-97-4	1.00	161.5	73	0.72	-2.44	2.83E-03	suspension	1.08	3.41E-02
Zopiclone	43200-80-2	0.98	178	73	2.71	-4.54	1.93E-05	suspension	3.08	2.33E-02
Zotepine	26615-21-4	1.00	90.5	73	5.43	-4.85	1.36E-03	suspension	2.11	1.75E-01
Zuclopenthixol	53772-83-1	0.95	84.5	73	3.91	-3.72	2.49E-04	suspension	2.91	2.01E-01
Acamprosate	77337-76-9	0.11	190	235	-2.68	0.39	1.10E-02	solution	0.21	1.77E-02
Acarbose	56180-94-0	0.02	95.6	181	-7.91	-0.96	4.65E-04	solution	2.52	1.56E-01

Acetaminophen	103-90-2	0.85	169.7	73	0.48	-1.01	1.98E-02	solution	0.15	2.82E-02
Acetanilide	103-84-4	1.00	114	73	1.24	-1.44	2.22E-03	solution	1.66	1.02E-01
Acipimox	51037-30-0	0.95	178.5	73	-1.00	0.33	4.87E-03	solution	0.68	2.31E-02
Acrivastine	87848-99-5	0.88	222	73	2.41	-3.12	9.18E-05	solution	1.97	8.47E-03
Adefovir	106941-25-7	0.16	250	73	-0.49	-1.70	3.66E-05	solution	2.08	4.45E-03
Albuterol	18559-94-9	0.83	151	73	0.69	-0.16	1.34E-04	solution	2.51	4.34E-02
Alendronic acid	66376-36-1	0.01	234	73	-0.73	0.34	1.61E-04	solution	1.60	6.43E-03
Alfentanil	71195-58-9	1.00	140.8	39	2.16	-3.77	3.53E-05	solution	3.19	5.49E-02
Alizapride	59338-93-1	1.00	139	73	0.84	-1.24	1.90E-03	solution	1.48	5.73E-02
Alprazolam	28981-97-7	0.90	228.2	73	1.92	-3.80	3.25E-05	solution	2.35	7.34E-03
Amifostine	20537-88-6	1.00	160.5	203	-1.23	-0.24	6.89E-03	solution	0.70	3.49E-02
Amikacin	37517-28-5	0.00	203.5	73	-5.26	0.23	1.54E-03	solution	0.93	1.30E-02
Amiloride	2609-46-3	0.50	241	73	0.93	-3.21	8.71E-05	solution	1.80	5.47E-03
Aminopyrine	58-15-1	1.00	108	73	0.85	-0.85	1.08E-03	solution	2.03	1.17E-01
Amphetamine	300-62-9	0.90	25	73	1.79	-1.42	4.44E-04	solution	3.25	7.91E-01
Amphotericin B	1397-89-3	0.03	170	73	2.30	-2.15	9.74E-05	solution	2.46	2.81E-02
Amrinone	60719-84-8	0.93	295.5	73	-0.21	-0.85	2.40E-04	solution	0.81	1.56E-03

Amygdalin	29883-15-6	0.05	220	73	-2.24	-1.72	1.09E-03	solution	0.91	8.87E-03
Anastrozole	120511-73-1	1.00	81.5	73	0.29	-3.26	3.42E-06	solution	4.80	2.15E-01
Antipyrine	60-80-0	0.98	112	73	0.44	-1.09	3.19E-03	solution	1.52	1.07E-01
Ascorbic Acid	50-81-7	1.00	191	73	-2.78	0.75	3.41E-02	solution	-0.29	1.73E-02
Atenolol	29122-68-7	0.50	147	73	0.34	-1.31	7.50E-04	solution	1.80	4.76E-02
Atropine	51-55-8	0.94	115	73	1.38	-2.06	2.76E-07	solution	5.56	9.95E-02
Azatadine	3964-81-6	0.90	125	73	2.69	-2.77	6.88E-06	solution	4.06	7.91E-02
Azithromycin	83905-01-5	0.60	114	73	2.58	-0.59	1.34E-03	solution	1.88	1.02E-01
Baclofen	1134-47-0	0.95	207	73	0.78	-1.64	3.73E-04	solution	1.51	1.20E-02
Benzydamine	642-72-8	0.87	140	74	3.56	-4.18	1.16E-05	solution	3.68	5.60E-02
Betahistine	5638-76-6	1.00	25	73	-0.02	0.07	3.52E-04	solution	3.35	7.91E-01
Betaxolol	63659-18-7	0.90	71	73	2.53	-2.57	1.30E-04	solution	3.32	2.74E-01
Betazole	105-20-4	1.00	25	73	-0.36	-0.68	2.70E-04	solution	3.47	7.91E-01
Biotin	58-85-5	1.00	232.5	73	0.86	-3.52	8.18E-07	solution	3.91	6.65E-03
Bromazepam	1812-30-2	0.84	237.7	73	2.28	-2.77	9.49E-05	solution	1.79	5.90E-03
Bromfenac	91714-94-2	1.00	129	153	2.02	-3.52	3.59E-07	solution	5.30	7.21E-02
Brompheniramine	86-22-6	0.89	25	73	3.24	-3.00	7.52E-05	solution	4.02	7.91E-01

Budesonide	51333-22-3	1.00	226.5	73	3.20	-4.66	6.03E-07	solution	4.10	7.64E-03
Busulfan	55-98-1	1.00	116	73	-0.56	-1.52	3.24E-05	solution	3.48	9.73E-02
Caffeine	58-08-2	0.99	238	73	-0.63	-0.52	3.09E-03	solution	0.28	5.86E-03
Calcitriol	32222-06-3	1.00	113	73	5.63	-5.62	7.20E-09	solution	7.16	1.04E-01
Captopril	62571-86-2	0.84	103.5	73	1.99	-2.04	2.07E-03	solution	1.80	1.30E-01
Carbimazole	22232-54-8	0.95	123.5	73	0.16	-1.20	3.22E-04	solution	2.40	8.18E-02
Carmustine	154-93-8	1.00	25	73	1.38	-1.70	2.33E-05	solution	4.53	7.91E-01
Carnitine	541-15-1	0.10	197	73	-4.52	0.46	4.91E-03	solution	0.49	1.51E-02
Ceftazidime	72558-82-8	0.00	136.5	84	-2.84	-0.64	1.46E-02	solution	0.62	6.07E-02
Chloral hydrate	302-17-0	1.00	57	73	0.99	-0.59	1.21E-02	solution	1.50	3.78E-01
Chlorambucil	305-03-3	1.00	65	73	2.61	-3.72	3.94E-05	solution	3.90	3.15E-01
Chlordiazepoxide	58-25-3	0.99	236.2	73	2.49	-0.68	3.34E-04	solution	1.26	6.11E-03
Chlorpheniramine	132-22-9	0.80	25	73	2.97	-2.96	2.90E-05	solution	4.43	7.91E-01
Chlorthalidone	77-36-1	0.65	225	73	0.70	-3.14	1.48E-04	solution	1.73	7.91E-03
Cidofovir	113852-37-2	0.03	260	73	-1.47	-1.09	1.07E-03	solution	0.52	3.53E-03
Cilazapril	88768-40-5	0.59	98	73	2.21	-3.72	2.40E-05	solution	3.79	1.47E-01
Cilazaprilat	90139-06-3	0.20	242	118	2.68	-3.80	2.57E-05	solution	2.32	5.34E-03

Clarithromycin	81103-11-9	1.00	218.5	73	2.81	-1.11	6.68E-04	solution	1.14	9.18E-03
Clavulanic acid	58001-44-8	0.75	117.5	151	-0.32	0.70	1.88E-03	solution	1.70	9.40E-02
Clenbuterol	37148-27-9	0.80	113	184	2.63	-2.80	2.16E-07	solution	5.68	1.04E-01
Clodronate	10596-23-3	0.03	250	73	-2.38	0.09	1.31E-02	solution	-0.47	4.45E-03
Clonidine	4205-90-7	0.95	130	73	2.36	-3.12	1.04E-05	solution	3.83	7.05E-02
Codeine	76-57-3	0.93	154	39	1.39	-2.31	1.20E-03	solution	1.53	4.05E-02
Corticosterone	50-22-6	1.00	181	73	1.95	-3.55	6.93E-06	solution	3.50	2.18E-02
Cotinine	486-56-6	0.97	25	73	0.08	-0.89	1.13E-04	solution	3.84	7.91E-01
Coumarin	91-64-5	1.00	69	73	1.39	-1.54	6.86E-04	solution	2.62	2.87E-01
Cyclopenthiazide	742-20-1	1.00	230	73	2.23	-4.15	3.95E-06	solution	3.25	7.05E-03
Cyclophosphamide	50-18-0	0.83	51	183	0.73	-0.80	1.15E-03	solution	2.58	4.34E-01
Cycloserine	68-41-7	0.72	156	73	-2.99	0.99	9.81E-03	solution	0.60	3.87E-02
Cyclosporine A	59865-13-3	0.33	149.5	73	2.79	-0.08	7.48E-04	solution	1.78	4.50E-02
Cymarin	508-77-0	0.47	148	73	0.66	-3.08	5.47E-06	solution	3.93	4.66E-02
Cysteamine	60-23-1	0.00	97.7	73	0.22	0.04	2.59E-02	solution	0.76	1.48E-01
Dalfampridine	504-24-5	1.00	158.5	39	0.34	-0.32	2.13E-04	solution	2.24	3.66E-02
Dapiprazole	72822-12-9	0.00	159	73	2.89	-4.17	7.68E-06	solution	3.67	3.61E-02

Desmethyldiazepam	1088-11-5	0.99	216.5	73	2.78	-3.55	3.69E-05	solution	2.42	9.61E-03
Desogestrel	54024-22-5	0.72	109.5	73	5.35	-5.41	4.83E-07	solution	5.37	1.13E-01
Desvenlafaxine Succinate	93413-62-8	0.81	223	141	1.74	-1.57	1.90E-04	solution	1.64	8.28E-03
Dextromoramide	357-56-2	1.00	182	73	2.53	-3.64	5.09E-05	solution	2.62	2.13E-02
Dextrose	50-99-7	0.99	146	73	-3.29	0.38	3.33E-02	solution	0.17	4.87E-02
Didanosine	69655-05-6	0.50	161.5	73	-1.43	-1.64	1.69E-03	solution	1.30	3.41E-02
Dienogest	65928-58-7	0.94	211.5	73	2.58	-3.89	6.42E-06	solution	3.23	1.08E-02
Diethylcarbamazine	90-89-1	0.90	48	73	1.66	-1.96	1.81E-03	solution	2.41	4.66E-01
Digitoxin	71-63-6	0.90	253.5	238	2.74	-4.44	1.57E-09	solution	6.42	4.10E-03
Digoxin	20830-75-5	0.78	247.5	73	1.29	-4.09	7.68E-10	solution	6.79	4.71E-03
Dihydrocodeine	125-28-0	0.89	112.5	73	0.61	-2.06	6.37E-04	solution	2.22	1.05E-01
Dipyridamole	58-32-2	0.58	163	73	3.35	-2.41	7.93E-04	solution	1.62	3.30E-02
Dofetilide	115256-11-6	1.00	148	73	1.38	-2.68	2.26E-06	solution	4.31	4.66E-02
Doxifluridine	9/5/3094	0.90	189.5	73	-0.72	-0.34	4.87E-03	solution	0.57	1.79E-02
Droxidopa	23651-95-8	0.90	233.5	73	-1.86	0.67	8.44E-03	solution	-0.11	6.50E-03
Dyphylline	479-18-5	0.95	158	73	-1.25	-0.26	1.42E-02	solution	0.42	3.70E-02
Edetic acid	60-00-4	0.05	240.5	73	-0.84	0.53	1.44E-02	solution	-0.41	5.53E-03

Eflornithine	70052-12-9	0.55	149.5	147	0.09	-0.01	1.32E-01	solution	-0.47	4.50E-02
Emtricitabine	143491-57-0	0.93	138	73	-0.27	-2.24	9.71E-04	solution	1.78	5.86E-02
Enalaprilat	76420-72-9	0.10	149.5	73	3.63	-2.96	5.74E-05	solution	2.89	4.50E-02
Entecavir	142217-69-4	1.00	220	73	-1.11	-2.39	3.61E-06	solution	3.39	8.87E-03
Ephedrine	299-42-3	0.97	38	73	1.08	-0.66	6.06E-04	solution	2.99	5.86E-01
Erythritol	149-32-6	0.90	121.5	73	-2.17	0.73	8.19E-04	solution	2.02	8.57E-02
Erythromycin	114-07-8	0.35	191.5	73	1.91	-1.30	5.45E-03	solution	0.50	1.71E-02
Estazolam	29975-16-4	0.93	228.5	73	2.52	-4.11	6.78E-06	solution	3.03	7.29E-03
Ethambutol	74-55-5	0.78	88.1	73	-0.29	0.46	7.34E-03	solution	1.40	1.85E-01
Ethinyl Estradiol	57-63-6	1.00	183	73	4.11	-4.89	1.01E-07	solution	5.31	2.08E-02
Ethionamide	536-33-4	0.90	165	73	1.17	-1.57	6.03E-03	solution	0.72	3.15E-02
Ethosuximide	77-67-8	0.93	64.5	73	0.25	-0.54	7.10E-03	solution	1.65	3.18E-01
Ethyl alcohol	64-17-5	1.00	25	73	-0.18	0.60	1.30E-01	solution	0.78	7.91E-01
Ethylmorphine	76-58-4	0.77	200	73	1.90	-2.66	1.66E-04	solution	1.93	1.41E-02
Etidronate	2809-21-4	0.05	195	144	-0.75	0.37	5.82E-03	solution	0.43	1.58E-02
Etilefrine	709-55-7	1.00	147.5	73	0.63	-0.32	2.76E-04	solution	2.23	4.71E-02
Etofylline	519-37-9	0.80	158	73	-0.91	-0.15	2.23E-03	solution	1.22	3.70E-02

Famotidine	76824-35-6	0.41	163.5	73	-1.66	-2.26	1.19E-04	solution	2.44	3.26E-02
Floxuridine	50-91-9	0.90	150.5	73	-1.41	-0.13	1.46E-04	solution	2.48	4.39E-02
Flucytosine	2022-85-7	1.00	296	73	-1.40	0.26	6.97E-02	solution	-1.66	1.54E-03
Fludrocortisone acetate	514-36-3	0.95	233.5	73	2.72	-4.66	2.37E-07	solution	4.44	6.50E-03
Flumazenil	78755-81-4	0.95	202	73	2.15	-3.85	9.89E-06	solution	3.13	1.34E-02
Flunisolide	3/3/3385	0.80	245	73	2.04	-4.00	1.47E-06	solution	3.53	4.99E-03
Flunitrazepam	1622-62-4	0.80	166.5	73	2.13	-4.10	6.38E-06	solution	3.68	3.04E-02
Folic Acid	59-30-3	0.75	250	73	-1.14	-2.89	1.81E-06	solution	3.39	4.45E-03
Fosfomycin	23155-02-4	0.36	94	73	-1.23	-0.03	2.17E-02	solution	0.87	1.61E-01
Fosmidomycin	66508-53-0	0.30	159	73	-1.63	0.21	6.55E-03	solution	0.74	3.61E-02
Frovatriptan	158747-02-5	0.40	140.5	123	0.93	-2.15	3.08E-05	solution	3.25	5.53E-02
Fructose	57-48-7	1.00	104	73	-1.03	-0.05	1.39E-01	solution	-0.03	1.28E-01
Gabapentin	60142-96-3	0.74	164	73	1.08	-0.80	7.01E-03	solution	0.66	3.22E-02
Galantamine	357-70-0	0.95	126.5	73	-0.05	-1.11	8.35E-05	solution	2.96	7.64E-02
Gemcitabine	95058-81-4	1.00	190	127	-2.22	-1.21	7.69E-03	solution	0.36	1.77E-02
Gentamicin C1	25876-10-2	0.00	97	73	-2.04	0.32	3.77E-04	solution	2.60	1.51E-01
Gentamicin C1a	26098-04-4	0.00	115.5	132	-2.93	0.35	4.00E-04	solution	2.39	9.84E-02

Gestodene	60282-87-3	1.00	197.9	73	2.02	-3.41	2.42E-07	solution	4.79	1.48E-02
Ginkgolide A	15291-75-5	0.90	300	73	-0.04	-1.82	8.81E-06	solution	2.20	1.41E-03
Ginkgolide B	15291-77-7	0.90	300	73	2.07	-2.64	8.48E-06	solution	2.22	1.41E-03
Gitoxin	4562-36-1	0.95	285	73	1.60	-4.20	1.92E-06	solution	3.01	1.99E-03
Glipizide	29094-61-9	1.00	208.5	73	1.88	-3.13	8.98E-05	solution	2.11	1.16E-02
Glyceryl1Nitrate	624-43-1	0.89	55	134	-0.51	0.05	2.92E-04	solution	3.13	3.96E-01
Glycine	56-40-6	1.00	233	73	-0.93	1.12	7.99E-02	solution	-1.08	6.58E-03
Granisetron	109889-09-0	1.00	153	98	2.91	-4.25	1.92E-06	solution	4.33	4.15E-02
Guanfacine	29110-47-2	1.00	226	73	1.33	-2.72	1.22E-05	solution	2.80	7.73E-03
Guanoxan	2165-19-7	0.50	164.5	73	0.83	-2.01	4.83E-05	solution	2.82	3.18E-02
Hydralazine	86-54-4	1.00	172.5	73	0.95	-2.02	1.25E-03	solution	1.33	2.65E-02
Hydrochlorothiazide	58-93-5	0.68	274	73	-0.02	-2.22	6.71E-04	solution	0.58	2.56E-03
Hydrocodone	125-29-1	0.80	197.5	73	2.57	-3.21	1.50E-04	solution	2.00	1.49E-02
Hydroflumethiazide	135-09-1	0.67	272.5	73	0.08	-2.33	6.03E-04	solution	0.64	2.65E-03
Hydromorphone	466-99-9	0.87	266.5	73	2.13	-2.74	8.41E-05	solution	1.56	3.04E-03
Hydroxyurea	127-07-1	1.00	134.5	73	-1.80	1.11	2.76E-02	solution	0.36	6.35E-02
Ifosfamide	3778-73-2	1.00	40	73	0.76	-0.80	7.66E-03	solution	1.86	5.60E-01

Imidapril	89371-37-9	0.70	139.5	73	2.28	-3.68	4.93E-05	solution	3.06	5.66E-02
Imipenem	64221-86-9	0.05	197	163	-2.95	-0.54	1.34E-02	solution	0.05	1.51E-02
Indacaterol maleate	312753-06-3	0.45	192	100	4.09	-4.64	7.64E-07	solution	4.34	1.69E-02
Indapamide	26807-65-8	0.90	161	73	1.96	-4.25	1.37E-05	solution	3.40	3.45E-02
Isocarboxazid	59-63-2	0.70	105.5	73	1.63	-2.62	2.59E-04	solution	2.68	1.24E-01
Isoniazid	54-85-3	0.80	260.5	73	-0.77	0.00	4.38E-03	solution	-0.10	3.49E-03
Isoproterenol	7683-59-2	0.85	155.5	73	0.32	-0.25	4.74E-05	solution	2.92	3.92E-02
Isosorbide dinitrate	87-33-2	0.90	70	73	0.95	-2.20	1.02E-03	solution	2.44	2.81E-01
Isosorbide-2-mononitrate	16051-77-7	1.00	89.7	221	-0.18	-0.74	6.28E-04	solution	2.45	1.78E-01
Kanamycin	59-01-8	0.01	165.5	207	-4.60	0.31	1.86E-03	solution	1.22	3.11E-02
Ketotifen	34580-13-7	0.90	152.5	73	2.19	-3.96	6.46E-06	solution	3.81	4.20E-02
K-Strophanthoside	33279-57-1	0.16	199.5	231	-2.74	-3.07	2.86E-07	solution	4.70	1.42E-02
Lacosamide	175481-36-4	1.00	143.5	73	0.73	-1.36	1.60E-03	solution	1.51	5.16E-02
Lamivudine	134678-17-4	0.86	161	73	-0.51	-1.96	1.31E-03	solution	1.42	3.45E-02
Lenalidomide	191732-72-6	0.90	265	105	-1.47	-1.17	9.64E-05	solution	1.51	3.15E-03
Letrozole	112809-51-5	1.00	182	73	0.43	-4.04	8.77E-06	solution	3.38	2.13E-02
Levamisole	14769-73-4	0.95	60.7	73	1.84	-2.92	2.45E-04	solution	3.15	3.47E-01

Levetiracetam	102767-28-2	1.00	117	73	-0.67	-0.83	2.12E-02	solution	0.65	9.50E-02
Levobunolol	47141-42-4	1.00	85	224	1.96	-2.72	4.56E-06	solution	4.64	1.99E-01
Levocetirizine	130018-77-8	0.85	112.5	73	1.62	-2.17	1.29E-05	solution	3.91	1.05E-01
Levodopa	59-92-7	0.86	277	73	-1.15	0.09	4.05E-02	solution	-1.23	2.39E-03
Levonorgestrel	797-63-7	1.00	236	73	3.37	-4.27	4.80E-06	solution	3.11	6.14E-03
Levosimendan	141505-33-1	0.90	212	73	2.07	-4.66	5.00E-06	solution	3.33	1.07E-02
Levothyroxine	51-48-9	0.60	235.5	73	4.72	-5.00	6.43E-07	solution	3.98	6.21E-03
Lidocaine	137-58-6	0.98	68.5	73	2.20	-2.21	1.28E-03	solution	2.36	2.90E-01
Liothyronine	2/3/6893	0.95	236.5	73	3.91	-4.38	1.54E-07	solution	4.60	6.07E-03
Lisinopril	76547-98-3	0.27	147	139	3.47	-2.96	9.86E-05	solution	2.68	4.76E-02
Lisuride	18016-80-3	1.00	186	73	3.21	-3.49	1.48E-05	solution	3.12	1.94E-02
Lodoxamide Trometamol	53882-12-5	0.70	212	73	-0.38	-3.46	3.21E-06	solution	3.52	1.07E-02
Lofexidine	31036-80-3	0.90	127	73	3.04	-3.85	9.26E-06	solution	3.91	7.55E-02
Loracarbef	76470-66-1	1.00	300	73	-1.60	-1.82	1.14E-03	solution	0.09	1.41E-03
Lorazepam	846-49-1	0.95	167	73	2.38	-3.44	3.12E-05	solution	2.98	3.01E-02
Lormetazepam	848-75-9	1.00	206	73	2.35	-3.60	5.97E-06	solution	3.31	1.22E-02
Lornoxicam	70374-39-9	1.00	227.5	73	0.77	-3.02	6.45E-05	solution	2.06	7.46E-03

Mannitol	69-65-8	0.19	167	73	-3.26	0.43	3.29E-01	solution	-1.04	3.01E-02
Mazindol	22232-71-9	0.93	216	73	2.36	-3.70	7.02E-06	solution	3.14	9.73E-03
Melagatran	159776-70-2	0.15	190	173	2.42	-4.35	6.33E-06	solution	3.45	1.77E-02
Memantine	19982-08-2	1.00	25	73	3.00	-2.68	1.12E-04	solution	3.85	7.91E-01
Meperidine	57-42-1	1.00	25	138	2.19	-1.82	3.64E-03	solution	2.34	7.91E-01
Mepindolol	23694-81-7	0.82	101	73	2.30	-1.96	5.72E-05	solution	3.38	1.37E-01
Mercaptopurine	50-44-2	0.50	313.5	73	-0.30	-2.17	9.86E-04	solution	0.02	1.03E-03
Mestranol	72-33-3	0.90	150.5	73	4.94	-5.40	1.60E-07	solution	5.44	4.39E-02
Metaproterenol	586-06-1	0.43	100	73	0.29	-0.24	3.79E-04	solution	2.57	1.41E-01
Metformin	657-24-9	0.54	119.5	192	-1.25	0.31	2.32E-02	solution	0.59	8.97E-02
Methimazole	60-56-0	0.95	147	73	-0.34	-0.36	5.26E-04	solution	1.96	4.76E-02
Methoxyamphetamine	64-13-1	0.80	209	133	1.68	-1.54	3.03E-05	solution	2.58	1.14E-02
Methyldopa	555-30-6	0.50	303	73	-0.74	-0.23	9.46E-03	solution	-0.86	1.31E-03
Methylergonovine	113-42-8	1.00	172	73	2.99	-3.04	2.36E-06	solution	4.06	2.68E-02
Methylphenidate	113-45-1	0.80	75	222	2.31	-2.12	2.57E-04	solution	2.99	2.50E-01
Methysergide	361-37-5	1.00	195	73	1.81	-2.74	1.70E-05	solution	2.97	1.58E-02
Metoclopramide	364-62-5	0.88	147.2	73	2.16	-2.52	2.00E-04	solution	2.37	4.74E-02

Metoprolol	37350-58-6	0.96	25	182	1.63	-1.38	1.50E-03	solution	2.72	7.91E-01
Metronidazole	443-48-1	0.95	159	73	-0.14	-0.77	1.17E-02	solution	0.49	3.61E-02
Mianserin	24219-97-4	0.70	110	219	1.14	-2.77	3.40E-04	solution	2.52	1.12E-01
Midodrine	42794-76-3	0.93	106.2	86	-0.27	-0.47	5.90E-05	solution	3.32	1.22E-01
Mifobate	76541-72-5	0.82	82.2	205	0.31	-1.28	1.67E-03	solution	2.10	2.12E-01
Miglitol	72432-03-2	1.00	114	73	-2.21	0.68	1.45E-03	solution	1.85	1.02E-01
Miglustat	72599-27-0	1.00	125.5	73	0.03	-0.19	1.37E-03	solution	1.76	7.82E-02
Milnacipran	92623-85-3	0.84	114.5	107	0.83	-1.41	8.12E-04	solution	2.09	1.01E-01
Milrinone	78415-72-2	0.83	300	73	1.27	-1.74	1.42E-05	solution	2.00	1.41E-03
Mirtazapine	61337-67-5	0.80	115	73	0.89	-2.37	1.70E-04	solution	2.77	9.95E-02
Misoprostol	59122-46-2	0.88	25	73	3.80	-4.01	2.09E-06	solution	5.58	7.91E-01
Moclobemide	71320-77-9	0.88	137	73	1.34	-1.62	2.23E-03	solution	1.43	6.00E-02
Modafinil	68693-11-8	0.80	165	73	1.18	-2.38	7.31E-04	solution	1.63	3.15E-02
Molsidomine	25717-80-0	1.00	140.5	73	-0.87	-0.76	1.65E-04	solution	2.53	5.53E-02
Morphine	57-27-2	0.90	253.5	73	0.87	-1.82	3.51E-04	solution	1.07	4.10E-03
Moxonidine	75438-57-2	0.88	218	73	0.33	-2.11	2.48E-06	solution	3.57	9.29E-03
Mycophenolate Mofetil	128794-94-5	0.96	93.5	73	3.69	-3.66	1.66E-02	solution	0.99	1.63E-01

N Acetylprocainamide	32795-44-1	0.83	139	229	1.51	-1.82	1.80E-03	solution	1.50	5.73E-02
Nadolol	42200-33-9	0.32	130	73	0.56	-1.74	2.07E-03	solution	1.53	7.05E-02
Nalbuphine	20594-83-6	1.00	230.5	73	1.00	-2.77	1.68E-04	solution	1.62	6.97E-03
Naloxone	465-65-6	0.91	177.5	73	1.78	-2.29	1.83E-05	solution	3.11	2.36E-02
Naratriptan	121679-13-8	0.70	170.5	73	1.15	-3.17	1.49E-05	solution	3.27	2.77E-02
Neomycin	1404-04-2	0.03	64.2	180	-2.78	-1.32	9.54E-03	solution	1.53	3.21E-01
Netilmicin	56391-56-1	0.00	101.5	185	-1.84	0.32	9.46E-04	solution	2.16	1.36E-01
Netivudine	84558-93-0	0.28	242.5	129	-0.49	-2.23	7.09E-04	solution	0.87	5.28E-03
Niacin	59-67-6	0.94	236.6	73	0.22	-0.29	6.09E-03	solution	0.00	6.05E-03
Nicorandil	65141-46-0	1.00	92.5	73	0.74	-1.12	1.89E-04	solution	2.95	1.67E-01
Nicotine	54-11-5	1.00	25	73	0.57	-0.42	4.93E-04	solution	3.20	7.91E-01
Nitrazepam	146-22-5	0.95	225	73	2.36	-3.54	7.10E-05	solution	2.05	7.91E-03
Nizatidine	76963-41-2	0.95	131	73	-0.49	0.48	9.05E-04	solution	1.88	6.89E-02
Nomifensine	24526-64-5	1.00	180	73	1.01	-2.15	8.38E-04	solution	1.42	2.23E-02
Nordazepam	1088-11-5	0.99	216.5	73	2.78	-3.55	3.69E-05	solution	2.42	9.61E-03
Norethindrone	68-22-4	1.00	203.5	73	2.86	-4.00	3.36E-06	solution	3.59	1.30E-02
Norfenfluramine	1886-26-6	0.85	25	73	2.63	-2.33	9.84E-05	solution	3.90	7.91E-01

Norgestrel	6533-00-2	1.00	208	73	3.37	-4.27	1.60E-06	solution	3.86	1.17E-02
Oseltamivir	196618-13-0	0.75	107.5	117	1.71	-1.85	4.80E-04	solution	2.39	1.18E-01
Oseltamivir Acid	187227-45-8	0.80	177.5	157	0.74	-1.59	1.06E-03	solution	1.35	2.36E-02
Ouabain	630-60-4	0.03	190	73	-2.21	-2.89	4.11E-05	solution	2.63	1.77E-02
Oxiracetam	62613-82-5	0.75	166.5	73	-2.48	0.62	5.06E-03	solution	0.78	3.04E-02
Oxprenolol	6452-71-7	0.95	79	73	2.15	-1.80	1.21E-03	solution	2.28	2.28E-01
Oxycodone	76-42-6	0.60	219	73	1.59	-2.24	1.01E-03	solution	0.95	9.08E-03
Palonosetron	135729-61-2	0.97	87.5	73	2.46	-3.32	8.43E-07	solution	5.35	1.87E-01
Pamidronic acid	40391-99-9	0.05	235	87	-0.89	0.60	3.83E-04	solution	1.21	6.28E-03
Paricalcitol	131918-61-1	0.86	174	158	5.90	-5.74	3.46E-08	solution	5.87	2.56E-02
Penciclovir	39809-25-1	0.10	276	73	-1.35	-1.92	3.95E-05	solution	1.79	2.44E-03
Pentoxifylline	5/6/6493	0.95	105	73	-0.15	-1.48	4.31E-03	solution	1.46	1.25E-01
Pergolide	66104-22-1	0.60	217.5	73	3.90	-3.70	9.54E-06	solution	2.99	9.40E-03
Perindopril	82834-16-0	0.95	112	92	4.10	-3.34	2.17E-05	solution	3.69	1.07E-01
Phencyclidine	77-10-1	0.95	46.2	73	4.25	-3.09	4.93E-05	solution	3.99	4.85E-01
Phenglutarimide	1156-05-4	1.00	126	73	1.89	-2.12	1.73E-04	solution	2.65	7.73E-02
Pheniramine	86-21-5	0.99	25	73	2.20	-2.18	1.56E-04	solution	3.70	7.91E-01

Phenobarbital	50-06-6	1.00	176	73	0.53	-2.27	5.58E-04	solution	1.64	2.44E-02
Phenylalanine	150-30-1	1.00	283	73	0.24	-0.72	3.63E-02	solution	-1.24	2.08E-03
Phenylpropanolamine	14838-15-4	0.95	101.2	73	0.36	-0.46	1.19E-03	solution	2.06	1.37E-01
Physostigmine	57-47-6	0.05	105.5	73	1.27	-1.52	3.64E-06	solution	4.53	1.24E-01
Pindolol	13523-86-9	0.90	172	73	1.68	-1.59	2.42E-04	solution	2.04	2.68E-02
Pirenzepine	28797-61-7	0.20	228	177	0.21	-2.49	4.27E-04	solution	1.24	7.38E-03
Piretanide	55837-27-9	0.85	226	73	2.30	-3.70	3.31E-05	solution	2.37	7.73E-03
Piroxicam	36322-90-4	1.00	199	73	0.59	-2.48	6.04E-05	solution	2.38	1.44E-02
Piroximone	84490-12-0	0.81	264.5	223	1.86	-2.35	2.30E-04	solution	1.14	3.18E-03
Pizotyline	15574-96-6	0.80	149.5	164	2.71	-3.59	1.02E-05	solution	3.65	4.50E-02
Polythiazide	346-18-9	1.00	202.5	73	2.05	-3.47	9.09E-06	solution	3.16	1.33E-02
Pomalidomide	19171-19-8	0.83	191.5	73	-0.71	-2.11	1.46E-05	solution	3.07	1.71E-02
Practolol	6673-35-4	0.95	135	73	0.59	-1.21	2.25E-03	solution	1.45	6.28E-02
Pramipexole	104632-26-0	0.80	118	106	2.35	-2.28	2.84E-05	solution	3.51	9.29E-02
Pregabalin	148553-50-8	0.90	187	73	1.09	-0.89	2.83E-03	solution	0.83	1.90E-02
Procyclidine	77-37-2	1.00	86	73	3.86	-3.14	6.95E-05	solution	3.45	1.94E-01
Prothionamide	14222-60-7	0.90	142	73	1.68	-1.92	2.77E-03	solution	1.28	5.34E-02

Proxyphylline	603-00-9	1.00	135.5	73	-0.56	-0.49	1.01E-02	solution	0.79	6.21E-02
Pseudoephedrine	90-82-4	1.00	118.4	73	1.08	-0.66	1.45E-03	solution	1.80	9.20E-02
Pyrazinamide	98-96-4	1.00	190	73	-0.71	0.26	1.46E-02	solution	0.08	1.77E-02
Quinagolide	87056-78-8	1.00	123.2	73	4.12	-4.60	2.28E-06	solution	4.56	8.24E-02
Quinalbarbitone	76-73-3	0.90	100	73	2.30	-0.48	1.26E-03	solution	2.05	1.41E-01
Raffinose	000512-69-6	0.00	118.5	73	-5.10	-0.70	1.59E-02	solution	0.76	9.18E-02
Ramelteon	196597-26-9	0.84	114	73	2.29	-3.51	3.08E-05	solution	3.52	1.02E-01
Ranitidine	66357-35-5	0.57	69.5	73	-0.07	0.14	9.54E-04	solution	2.47	2.84E-01
Reboxetine	71620-89-8	1.00	170.5	73	2.45	-2.96	3.83E-05	solution	2.86	2.77E-02
Riboflavin	83-88-5	0.80	280	73	0.10	-3.15	7.97E-05	solution	1.45	2.23E-03
Rimiterol	32953-89-2	0.48	203.5	73	0.74	-0.54	2.15E-05	solution	2.78	1.30E-02
Risedronic acid	105462-24-6	0.01	241	162	0.55	-0.70	1.77E-05	solution	2.49	5.47E-03
Ritodrine	26652-09-5	0.95	89	73	2.04	-1.96	4.18E-04	solution	2.64	1.81E-01
Rivastigmine	123441-03-2	0.98	25	73	2.06	-1.00	4.79E-05	solution	4.22	7.91E-01
Rizatriptan	144034-80-0	0.90	120.5	73	1.20	-2.24	1.11E-04	solution	2.90	8.77E-02
Rofecoxib	162011-90-7	0.93	209	39	-0.34	-2.52	1.59E-04	solution	1.86	1.14E-02
Ropinirole	91374-21-9	0.98	242	142	2.49	-2.42	9.22E-05	solution	1.76	5.34E-03

Roquinimex	84088-42-6	1.00	202	73	1.03	-2.20	1.62E-05	solution	2.92	1.34E-02
Rosuvastatin	287714-41-4	0.50	112	171	0.89	-3.44	8.31E-05	solution	3.11	1.07E-01
Salicylic Acid	69-72-7	1.00	159	73	2.01	-1.36	1.81E-04	solution	2.30	3.61E-02
Saxagliptin	361442-04-8	0.75	109	131	0.20	-2.96	1.59E-05	solution	3.86	1.14E-01
Scopolamine	51-34-3	0.93	25	73	0.69	-2.22	6.53E-08	solution	7.08	7.91E-01
Selegiline	14611-51-9	1.00	25	73	2.68	-2.41	5.35E-05	solution	4.17	7.91E-01
Sirolimus	53123-88-9	0.90	184	73	4.26	-3.57	8.86E-06	solution	3.36	2.03E-02
Sorivudine	77181-69-2	0.82	182	73	-0.03	-2.52	4.30E-04	solution	1.69	2.13E-02
Stavudine	3056-17-5	1.00	165.5	73	-0.65	-1.70	3.57E-04	solution	1.94	3.11E-02
Streptozocin	18883-66-4	0.00	115	73	-1.33	-0.77	2.44E-02	solution	0.61	9.95E-02
Sufentanil	56030-54-7	0.90	96.6	73	3.95	-3.42	3.88E-06	solution	4.59	1.52E-01
Sumatriptan	103628-46-2	0.67	170	73	0.44	-2.52	4.06E-05	solution	2.84	2.81E-02
Tamsulosin	106133-20-4	1.00	121	109	2.14	-3.62	1.95E-06	solution	4.65	8.67E-02
Temazepam	846-50-4	0.95	120	73	2.19	-3.03	4.99E-05	solution	3.25	8.87E-02
Temozolomide	85622-93-1	1.00	212	73	-1.27	-1.89	1.67E-03	solution	0.81	1.07E-02
Tenoxicam	59804-37-4	1.00	211	73	0.01	-2.40	5.93E-05	solution	2.27	1.09E-02
Terazosin	63590-64-7	0.91	273.3	73	0.80	-3.64	5.16E-05	solution	1.70	2.60E-03

Terbutaline	23031-25-6	0.63	120.5	73	0.70	-0.55	6.66E-05	solution	3.12	8.77E-02
Tesaglitazar	251565-85-2	1.00	84	159	1.55	-3.47	2.45E-06	solution	4.92	2.03E-01
Theophylline	58-55-9	1.00	272	73	-0.28	-1.14	2.89E-03	solution	-0.03	2.68E-03
Tibolone	5630-53-5	0.90	167	73	3.52	-4.38	8.01E-06	solution	3.57	3.01E-02
Timolol	26839-75-8	0.95	72	73	1.28	-2.85	1.90E-04	solution	3.15	2.68E-01
Tobramycin	32986-56-4	0.00	217	128	-4.22	0.33	1.16E-03	solution	0.92	9.50E-03
Tolazoline	59-98-3	0.90	66	179	1.80	-2.25	7.49E-04	solution	2.61	3.08E-01
Toliprolol	2933-94-0	0.90	75.5	73	1.80	-1.42	1.34E-03	solution	2.26	2.47E-01
Tolmesoxide	38452-29-8	0.98	92.5	75	0.41	-1.48	1.87E-03	solution	1.95	1.67E-01
Tranexamic acid	1197-18-8	0.55	389	73	0.50	-0.57	2.48E-02	solution	-2.14	1.81E-04
Triazolam	28911-01-5	0.85	234	73	2.08	-4.21	1.46E-06	solution	3.64	6.43E-03
Trihexyphenidyl	144-11-6	1.00	114.7	73	4.39	-3.35	4.98E-05	solution	3.30	1.00E-01
Trofosfamide	22089-22-1	1.00	50.5	73	2.44	-2.14	9.27E-04	solution	2.68	4.39E-01
Tropisetron	89565-68-4	0.95	201.5	73	3.03	-3.19	1.76E-05	solution	2.89	1.36E-02
Urapidil	34661-75-1	0.78	157	73	1.64	-2.11	6.19E-04	solution	1.79	3.78E-02
Varenicline tartrate	249296-44-4	0.92	138	210	1.01	-2.03	9.47E-06	solution	3.79	5.86E-02
Venlafaxine	93413-69-5	0.95	103	73	2.48	-2.12	1.35E-03	solution	1.99	1.31E-01

Vigabatrin	60643-86-9	1.00	209	73	-0.30	0.10	2.32E-02	solution	-0.31	1.14E-02
Vildagliptin	274901-16-5	0.85	139	73	0.17	-2.00	3.30E-04	solution	2.24	5.73E-02
Viloxazine	46817-91-8	0.99	178	143	1.24	-1.49	1.90E-03	solution	1.09	2.33E-02
Xamoterol	81801-12-9	0.07	175.5	80	-0.70	-1.96	1.18E-03	solution	1.32	2.47E-02
Ximoprofen	56187-89-4	0.98	178	73	2.10	-2.72	1.15E-04	solution	2.31	2.33E-02
Zalcitabine	7481-89-2	0.85	209.5	73	-1.36	-1.00	1.07E-05	solution	3.03	1.13E-02
Zanamivir	139110-80-8	0.02	256	73	-1.87	-1.35	6.01E-05	solution	1.81	3.87E-03
Zidovudine	30516-87-1	0.97	109	73	-0.53	-1.32	2.25E-03	solution	1.71	1.14E-01
Zolmitriptan	139264-17-8	0.92	140	73	0.46	-2.70	3.48E-05	solution	3.21	5.60E-02
Zolpidem	82626-48-0	0.95	196	73	3.09	-3.38	3.25E-05	solution	2.68	1.54E-02

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